



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 09:49 PM EST

PDB ID : 6DQZ
EMDB ID : EMD-7986
Title : Class 4 IP3-bound human type 3 1,4,5-inositol trisphosphate receptor
Authors : Hite, R.K.; Paknejad, N.
Deposited on : 2018-06-11
Resolution : 6.01 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

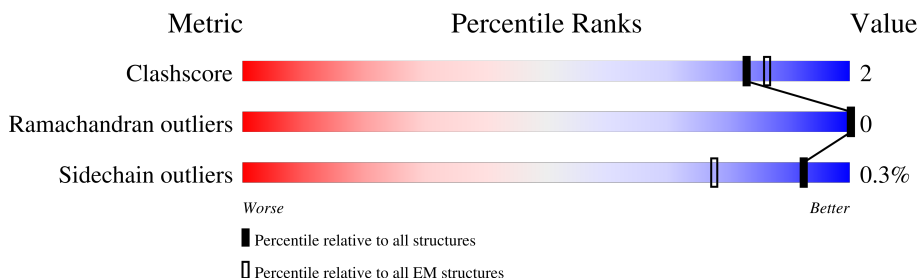
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2671	
1	B	2671	
1	C	2671	
1	D	2671	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 139662 atoms, of which 69852 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

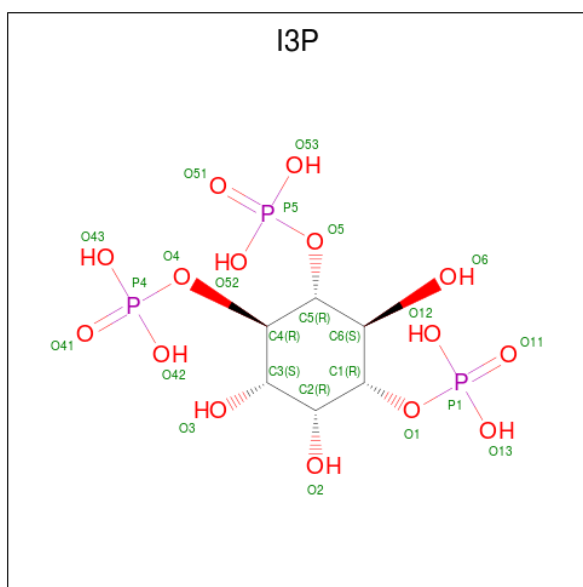
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2188	35064	11176	17554	3000	3228	106	0	0
1	B	2188	35064	11176	17554	3000	3228	106	0	0
1	D	2186	34699	11058	17354	2985	3199	103	0	0
1	C	2186	34699	11058	17354	2985	3199	103	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
2	A	1	1	1	0
2	B	1	1	1	0
2	D	1	1	1	0
2	C	1	1	1	0

- Molecule 3 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).

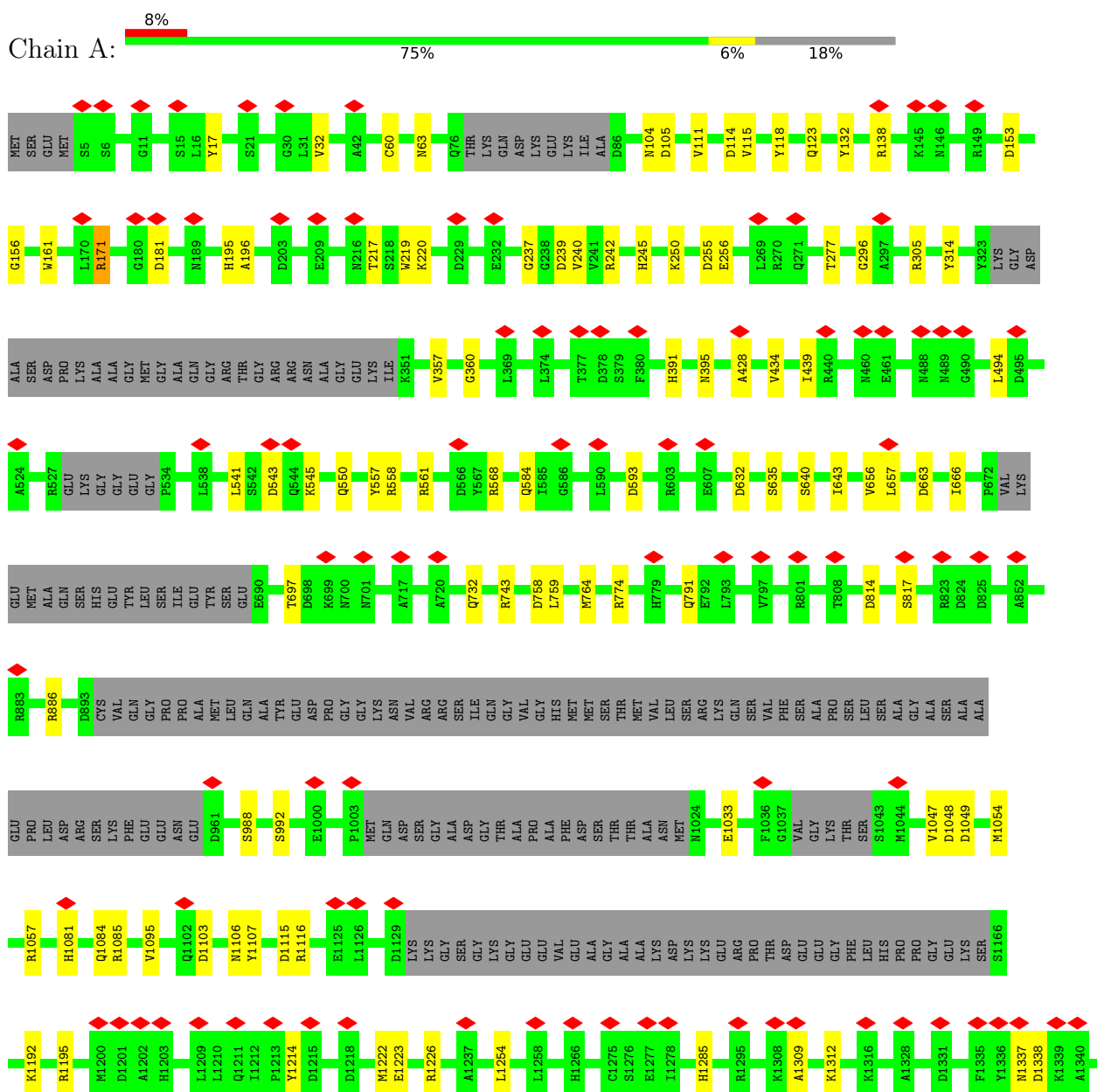


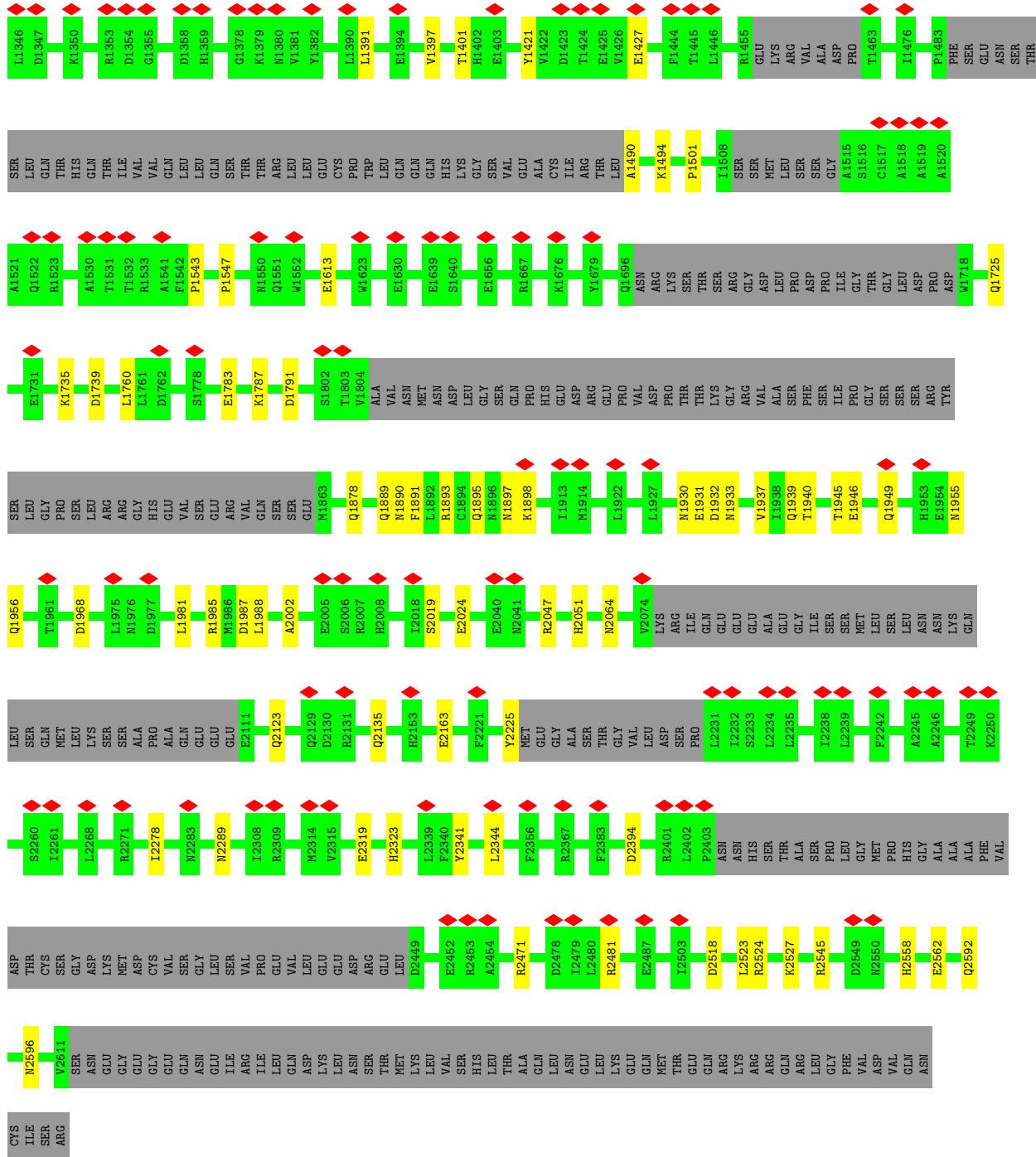
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
3	A	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	B	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	D	1	Total	C	H	O	P	0
			33	6	9	15	3	
3	C	1	Total	C	H	O	P	0
			33	6	9	15	3	

3 Residue-property plots

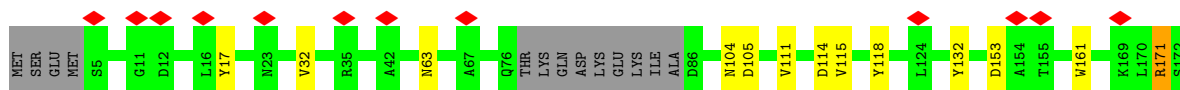
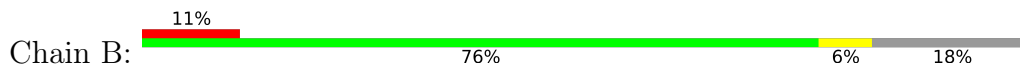
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

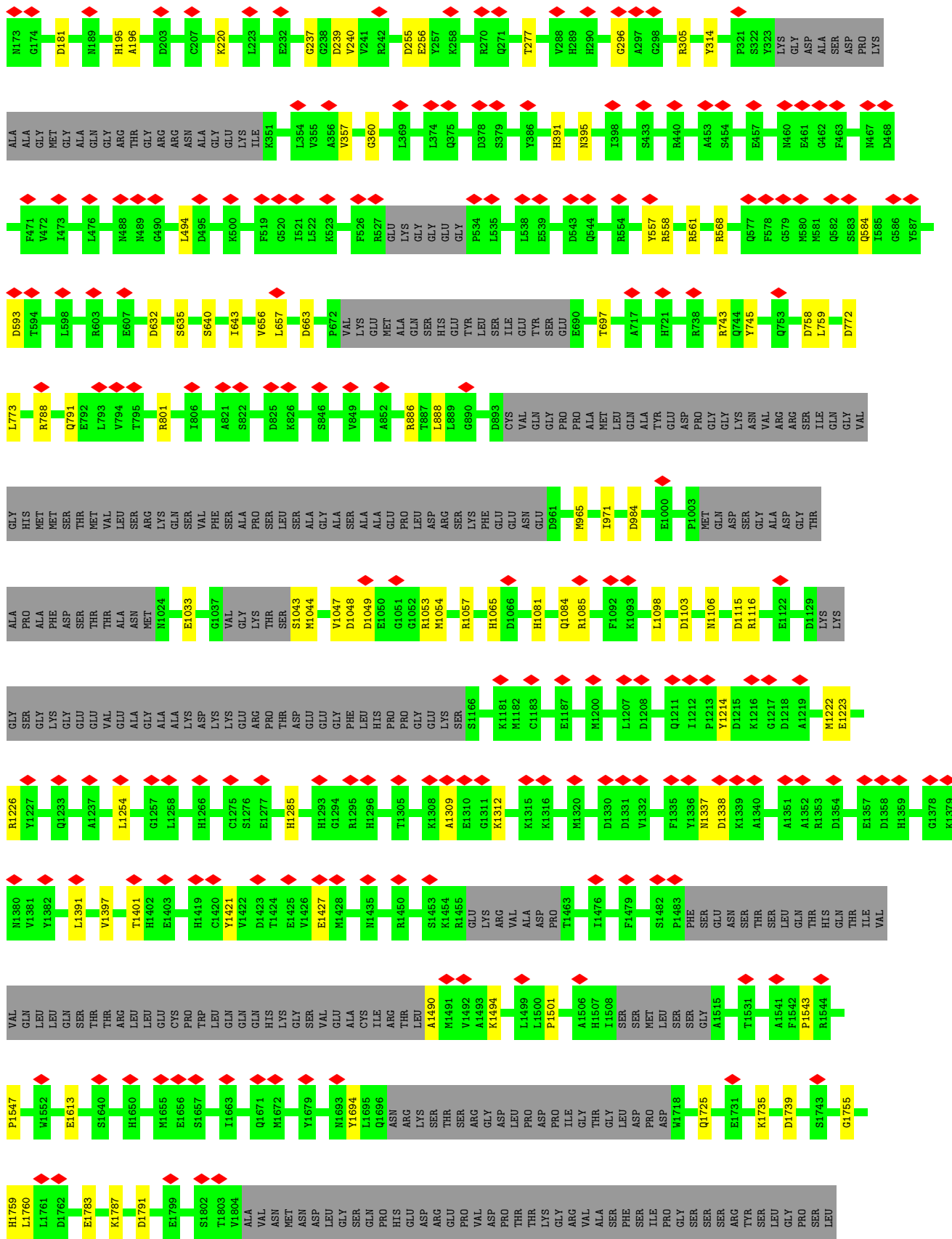
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

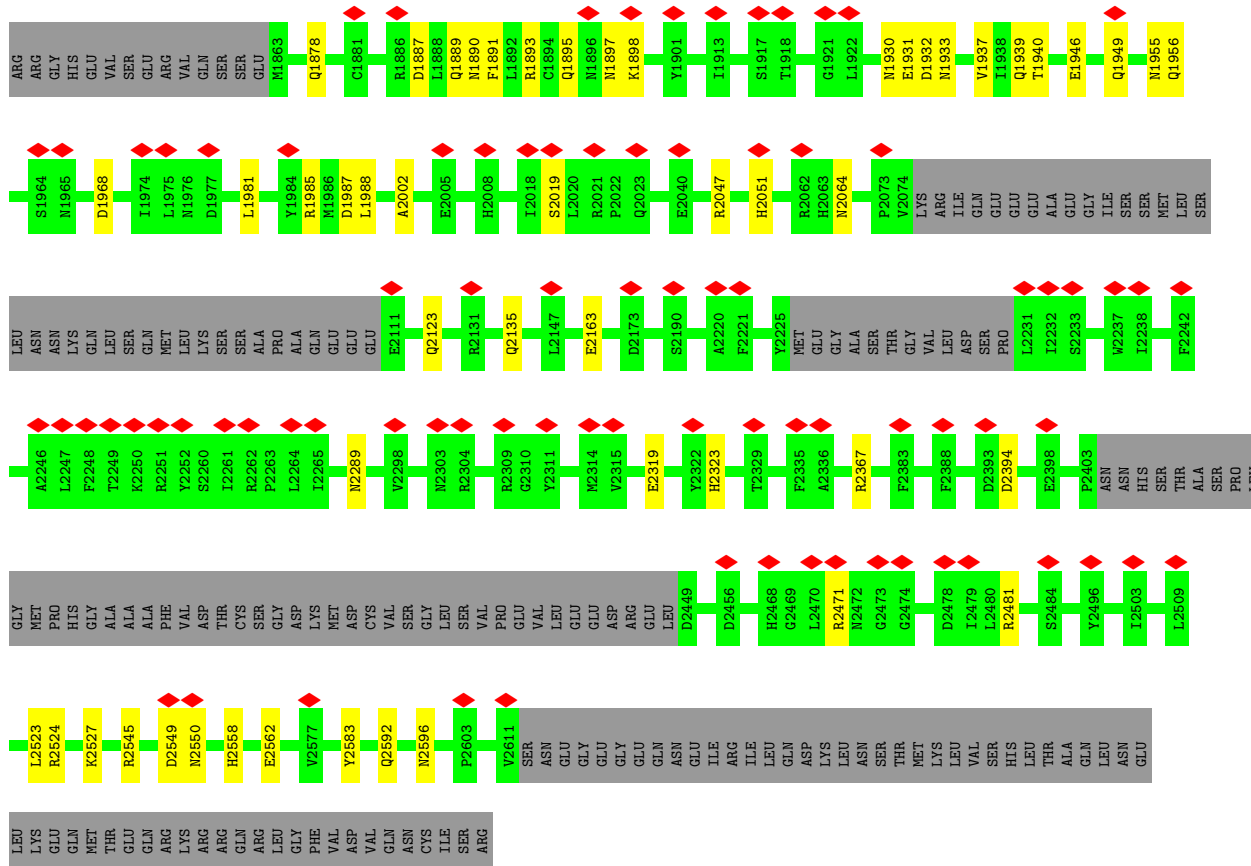




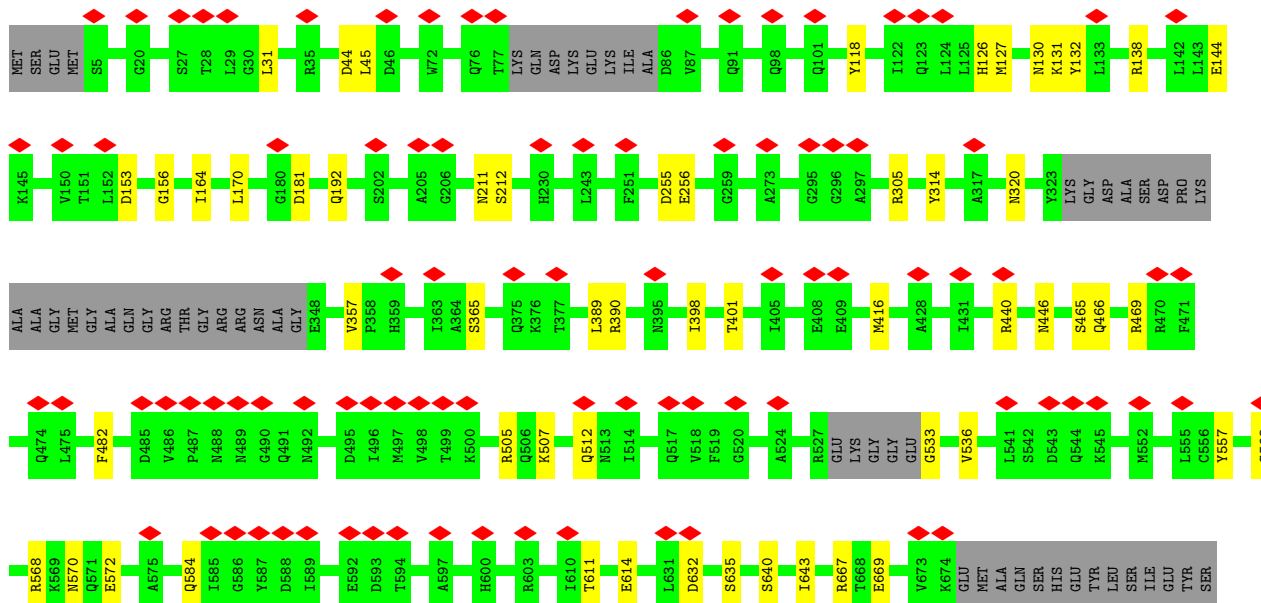
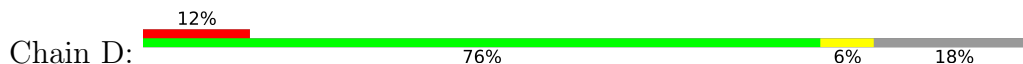
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

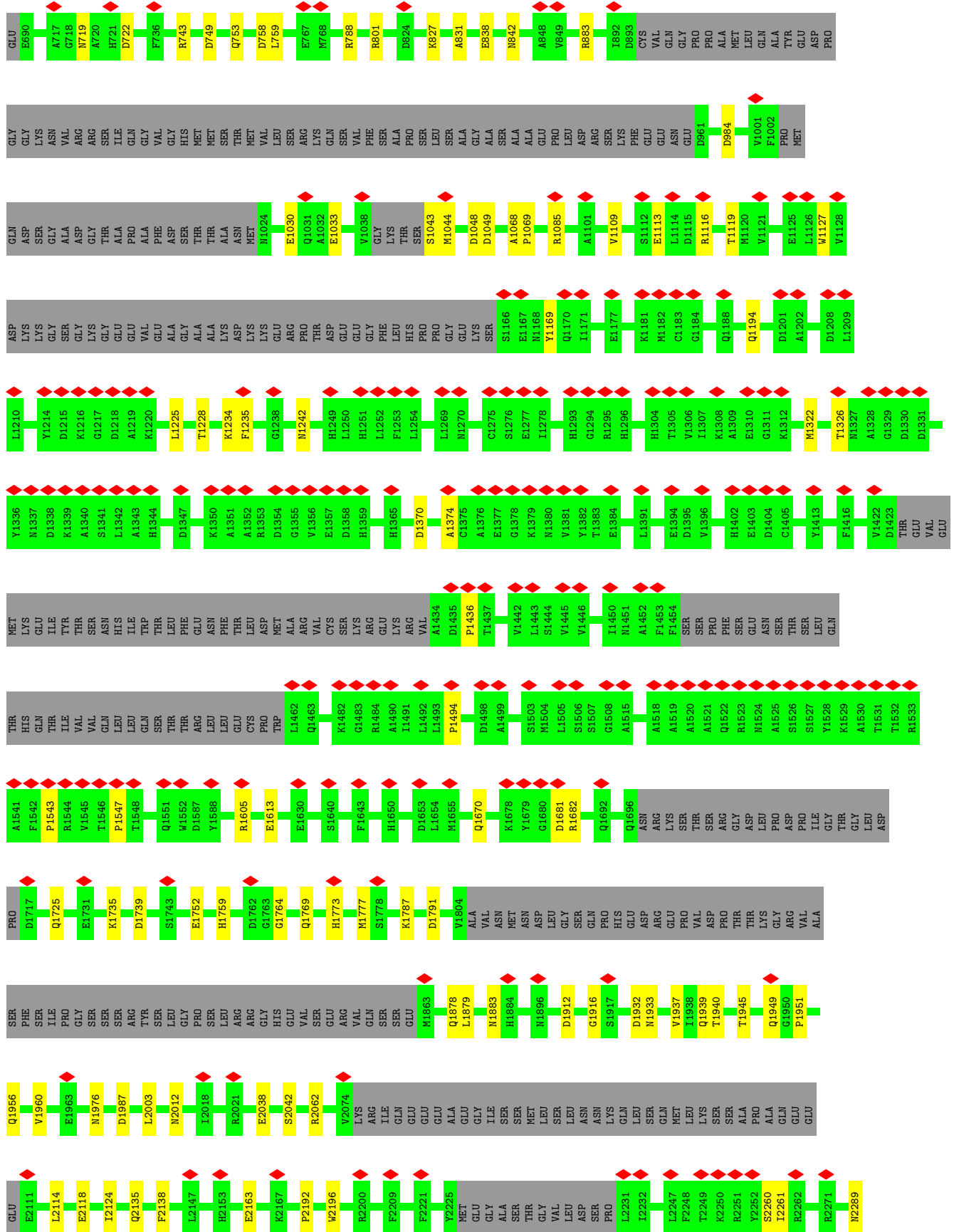


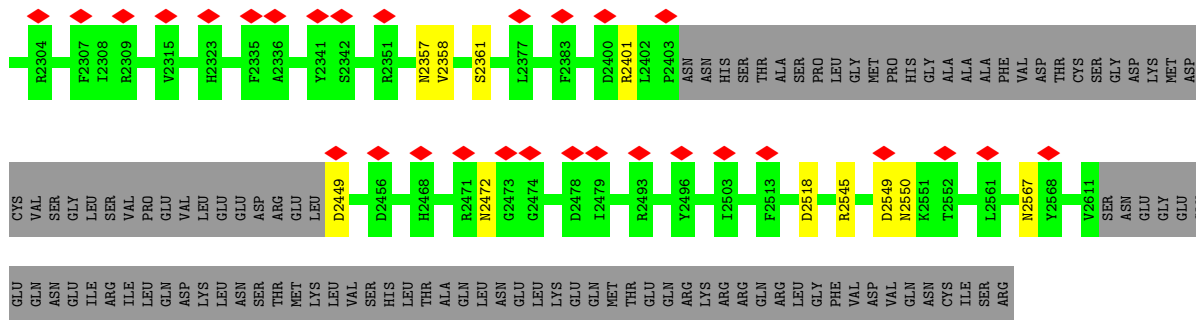




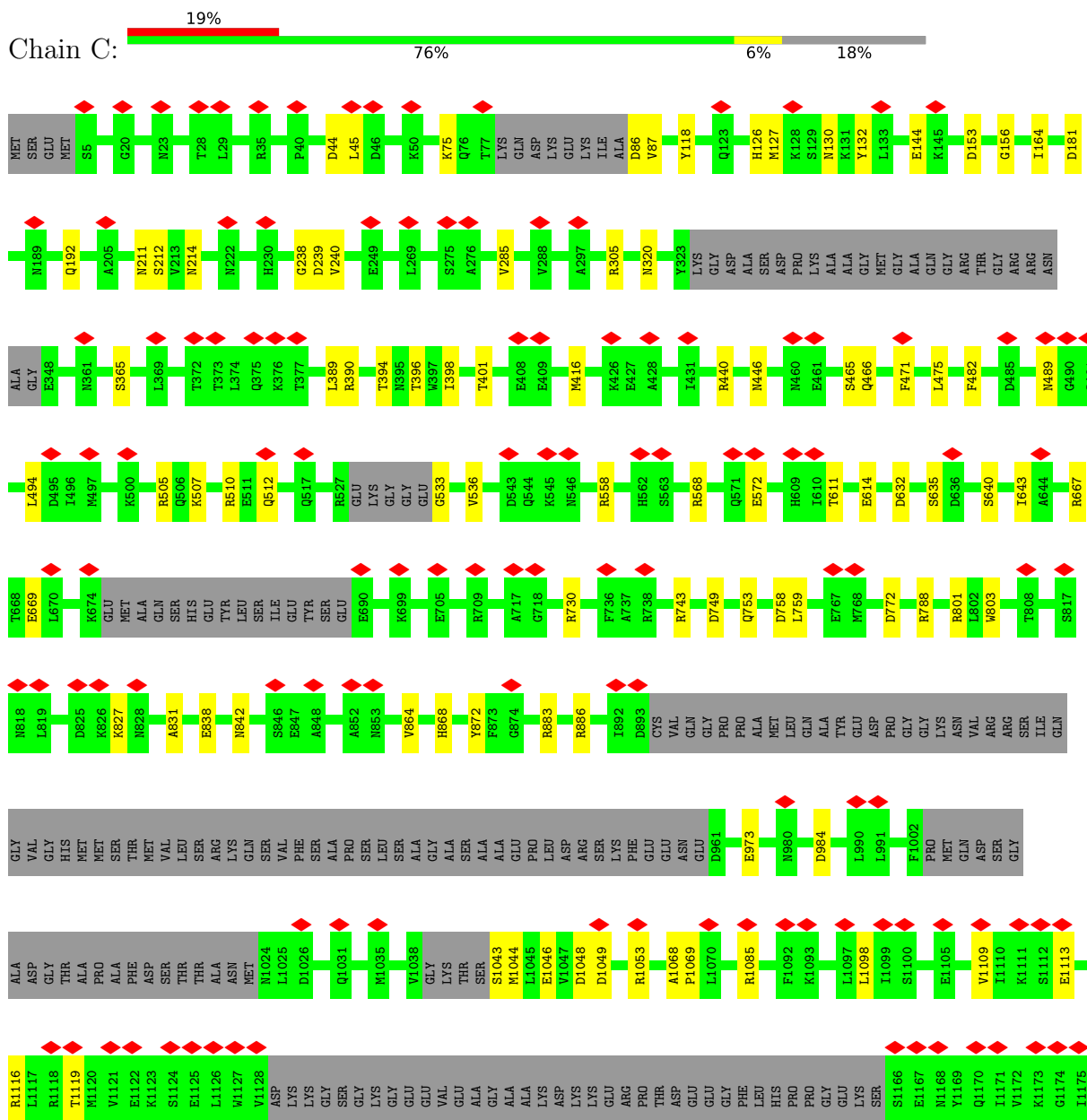
● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



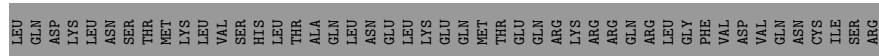




● Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3



L1176	E1177	R1178	L1179	M1180	K1181	M1182	C1183	G1184	V1185	E1186	E1187	Q1188	M1189	K1192	Q1193	L1196	M1199	M1200	D1201	A1202	V1205	M1206	L1207	D1208	L1209	L1210	Q1211	I1212	P1213	V1214	D1215	K1216	G1217	D1218	A1219	K1220	M1221	M1222	E1223	I1224	F1231	K1234	F1235	C1236	A1237	G1238	M1239	M1242	L1246	H1247	K1248							
H1249	H1250	H1251	L1252	F1253	L1254	T1255	P1256	G1257	L1258	E1262	T1263	M1264	Q1265	H1266	L1269	N1270	Q1273	L1274	C1275	S1276	E1277	I1278	S1279	E1280	P1281	V1282	L1283	Q1284	I1285	F1286	V1287	H1288	L1289	H1293	G1294	R1295	H1296	V1297	D1301	F1302	L1303	H1304	T1305	V1306	I1307	K1308	A1309	E1310	G1311	K1312	Y1313	V1314	K1315	K1316				
C1317	Q1318	D1319	M1320	I1321	M1322	T1323	E1324	L1325	T1326	M1327	A1328	G1329	D1330	D1331	V1332	V1333	F1335	M1337	D1338	K1339	A1340	S1341	L1342	A1343	H1344	L1345	L1346	D1347	M1348	M1349	K1350	A1351	A1352	R1353	D1354	G1355	V1356	E1357	D1358	H1359	S1360	P1361	L1362	M1363	Y1364	H1365	I1366	S1367	D1370	L1371	L1372	A1373	A1374	C1375	A1376	E1377		
G1378	K1379	M1380	V1381	Y1382	T1383	E1384	I1385	K1386	C1387	T1388	S1389	L1390	L1391	P1392	L1393	E1394	D1395	V1396	S1398	V1399	V1400	T1401	H1402	E1403	D1404	C1405	I1406	T1407	E1408	V1409	K1410	M1411	M1415	F1416	V1417	H1418	H1419	C1420	Y1421	V1422	D1423	THR	GLU	VAL	L1362	M1363	Y1364	H1365	I1366	THR	TYR	THR	ASN	ASN	HIS	ILE	TRP	THR
LEU	PHE	GLU	ASN	THR	LEU	ASP	ALA	ARG	VAL	SER	LYS	ARG	GLU	ARG	VAL	A1434	D1435	P1436	T1437	L1438	E1439	K1440	Y1441	V1442	L1443	V1444	V1445	L1446	L1447	D1448	T1449	I1450	M1451	A1452	F1453	F1454	SER	SER	PRO	PHE	GLU	ASN	SER	THR	SER	LEU	GLN	THR	GLU	THR	GLN	HIS	GLN	THR	ILE	VAL	VAL	
GLN	LEU	GLN	SER	THR	THR	ARG	LEU	LEU	GLU	CYS	PRO	TRP	L1462	Q1463	Q1464	V1470	E1471	A1472	C1473	I1474	R1475	T1476	L1477	M1478	A1479	V1480	A1481	K1482	G1483	R1484	A1490	I1491	L1492	L1493	P1494	M1495	D1496	L1497	D1498	A1499	H1500	I1501	S1502	S1503	M1504	L1505	L1506	S1507	G1508	A1515	S1516	C1517	A1518	A1519	A1520	A1521	Q1522	
R1523	M1524	A1525	S1526	S1527	Y1528	K1529	A1530	T1531	C1532	R1533	A1541	F1542	P1543	R1544	V1545	T1546	T1548	A1549	M1550	Q1551	M1552	D1557	I1559	I1592	E1593	E1613	L1629	E1630	G1631	E1639	S1640	F1643	E1656	M1672	L1673	K1676	T1677	D1681	R1682	M1693	Q1696	ASN	ARG	LYS	SER	THR	SER											
ARG	GLY	ASP	LEU	PRO	ASP	PRO	ILE	THR	GLY	THR	LEU	LEU	ASP	PRO	D1717	W1718	Q1725	E1731	K1735	D1739	I1749	S1753	H1759	G1764	Q1769	S1778	S1802	T1803	V1804	ALA	VAL	ASN	ASN	ASN	ASP	LEU	GLY	SER	GLN	PRO	HIS	GLU	ASP	ARG	GLU	PRO	PRO	VAL	VAL	ASP	PRO							
THR	THR	LYS	GLY	ARG	VAL	ALA	SER	PHE	LEU	ILE	PRO	GLY	SER	SER	SER	SER	ARG	ARG	ARG	GLY	HIS	GLU	VAL	SER	GLU	M1863	Q1878	L1879	M1883	H1884	M1885	R1886	M1896	M1897	K1898	D1912	I1913	G1916	G1921	L1922																		
L1925	I1929	D1932	M1933	V1937	T1938	Q1939	T1940	T1945	Q1949	G1950	P1951	G1952	H1953	Q1956	H1962	E1963	S1964	M1965	G1966	M1976	D1977	D1987	E2005	S2006	R2007	H2008	S2019	L2020	R2021	E2038	R2039	E2040	M2041	S2042	R2062	P2073	V2074	LYS	ARG	ILE	ILE	GLU	GLU	ALA														
GLU	GLY	ILE	SER	MET	LEU	SER	ASN	ASN	GLN	MET	LEU	LYS	SER	SER	ALA	PRO	ALA	GLN	GLU	GLU	E2111	L2114	E2118	Q2123	T2124	Q2129	E2134	Q2135	F2138	H2153	E2163	K2167	P2192	W2196	F2209	F2214	A2220	F2221																				
Y2225	GLU	GLY	ALA	SER	THR	GLY	VAL	LEU	ASP	SER	PRO	L2231	L2232	S2233	L2234	L2235	F2236	W2237	I2238	L2239	I2240	C2241	F2242	L2247	F2248	T2249	K2250	R2251	Y2252	S2260	I2261	L2282	W2289	I2294	R2304	R2309	M2314	V2315	M2316	D2317	M2318	L2332	F2335	A2336	L2339	F2340	Y2341											
S2342	I2343	E2352	M2357	V2362	A2376	L2377	Q2393	D2394	D2400	F2403	ASN	ASN	HIS	SER	THR	ALA	SER	PRO	GLU	GLU	LEU	GLY	MET	PRO	HIS	GLY	ALA	ALA	ALA	PHE	VAL	ASP	THR	CYS	GLY	SER	GLY	ASP	LYS	MET	CYS	CYS	VAL	SER	GLY	LEU	SER	VAL	PRO	GLU	VAL	LEU	GLU	GLU	ASP			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	Not provided	
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.174	Depositor
Minimum map value	-4.203	Depositor
Average map value	-0.013	Depositor
Map value standard deviation	0.490	Depositor
Recommended contour level	1.96	Depositor
Map size (Å)	417.79202, 417.79202, 417.79202	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.088, 1.088, 1.088	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, I3P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/17827	0.47	3/24087 (0.0%)
1	B	0.26	0/17827	0.47	3/24087 (0.0%)
1	C	0.25	0/17650	0.46	4/23851 (0.0%)
1	D	0.25	0/17650	0.46	4/23851 (0.0%)
All	All	0.26	0/70954	0.47	14/95876 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1501	PRO	N-CA-CB	5.70	110.14	103.30
1	B	1547	PRO	N-CA-CB	5.67	110.10	103.30
1	C	1494	PRO	N-CA-CB	5.65	110.08	103.30
1	A	1547	PRO	N-CA-CB	5.62	110.04	103.30
1	D	1547	PRO	N-CA-CB	5.61	110.03	103.30
1	C	1547	PRO	N-CA-CB	5.60	110.02	103.30
1	B	1543	PRO	N-CA-CB	5.59	110.01	103.30
1	D	1543	PRO	N-CA-CB	5.58	109.99	103.30
1	C	1543	PRO	N-CA-CB	5.58	109.99	103.30
1	A	1543	PRO	N-CA-CB	5.55	109.96	103.30
1	D	1494	PRO	N-CA-CB	5.55	109.95	103.30
1	C	1436	PRO	N-CA-CB	5.55	109.96	103.30
1	A	1501	PRO	N-CA-CB	5.54	109.95	103.30
1	D	1436	PRO	N-CA-CB	5.44	109.83	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17510	17554	17452	94	0
1	B	17510	17554	17452	83	0
1	C	17345	17354	17182	83	0
1	D	17345	17354	17182	84	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	9	9	2	0
3	B	24	9	9	1	0
3	C	24	9	9	2	0
3	D	24	9	9	1	0
All	All	69810	69852	69304	333	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:MET:SD	1:A:1057:ARG:NH2	2.61	0.73
1:B:2163:GLU:O	1:C:2545:ARG:NH1	2.21	0.73
1:B:743:ARG:NH2	1:B:791:GLN:O	2.23	0.71
1:D:192:GLN:O	1:D:212:SER:OG	2.08	0.71
1:C:749:ASP:O	1:C:753:GLN:NE2	2.23	0.71
1:B:557:TYR:OH	1:B:584:GLN:OE1	2.09	0.70
1:A:2545:ARG:NH1	1:D:2163:GLU:O	2.25	0.70
1:A:557:TYR:OH	1:A:584:GLN:OE1	2.10	0.70
1:C:1987:ASP:OD1	1:C:2042:SER:OG	2.08	0.70
1:D:507:LYS:NZ	3:D:3002:I3P:O53	2.25	0.69
1:B:1054:MET:SD	1:B:1057:ARG:NH2	2.65	0.69
1:B:171:ARG:NH1	1:B:181:ASP:OD2	2.26	0.69
1:A:171:ARG:NH1	1:A:181:ASP:OD2	2.26	0.68
1:D:144:GLU:OE2	1:D:211:ASN:ND2	2.26	0.68
1:D:1725:GLN:NE2	1:D:1759:HIS:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1085:ARG:NH1	1:A:1613:GLU:OE2	2.27	0.68
1:C:2062:ARG:NH1	1:C:2135:GLN:OE1	2.27	0.68
1:B:1937:VAL:O	1:B:1940:THR:OG1	2.11	0.68
1:C:192:GLN:O	1:C:212:SER:OG	2.12	0.68
1:B:1214:TYR:OH	1:B:1222:MET:SD	2.48	0.68
1:A:561:ARG:NH1	1:A:593:ASP:O	2.27	0.68
1:B:1391:LEU:O	1:B:1421:TYR:OH	2.13	0.67
1:D:1987:ASP:OD1	1:D:2042:SER:OG	2.07	0.67
1:A:2524:ARG:NE	1:D:2518:ASP:OD2	2.23	0.67
1:D:2545:ARG:NH1	1:C:2163:GLU:O	2.27	0.67
1:C:1937:VAL:O	1:C:1940:THR:OG1	2.10	0.67
1:D:1937:VAL:O	1:D:1940:THR:OG1	2.10	0.66
1:D:2062:ARG:NH1	1:D:2135:GLN:OE1	2.28	0.66
1:A:886:ARG:NH1	1:A:1047:VAL:O	2.28	0.66
1:C:144:GLU:OE2	1:C:211:ASN:ND2	2.29	0.66
1:A:1391:LEU:O	1:A:1421:TYR:OH	2.12	0.66
1:B:1735:LYS:NZ	1:B:1739:ASP:OD2	2.29	0.66
1:A:1214:TYR:OH	1:A:1222:MET:SD	2.48	0.66
1:A:2163:GLU:O	1:B:2545:ARG:NH1	2.28	0.66
1:A:1735:LYS:NZ	1:A:1739:ASP:OD2	2.29	0.65
1:C:827:LYS:O	1:C:831:ALA:N	2.30	0.65
1:C:305:ARG:NH2	1:C:365:SER:OG	2.29	0.64
1:D:305:ARG:NH2	1:D:365:SER:OG	2.31	0.64
1:D:568:ARG:NH2	1:D:572:GLU:OE2	2.31	0.64
1:C:507:LYS:NZ	3:C:3002:I3P:O53	2.29	0.64
1:A:1103:ASP:OD2	1:A:1192:LYS:NZ	2.23	0.64
1:D:1235:PHE:O	1:D:1242:ASN:ND2	2.31	0.64
1:D:611:THR:OG1	1:D:614:GLU:OE1	2.08	0.63
1:C:801:ARG:NH2	1:C:984:ASP:OD1	2.31	0.63
1:A:743:ARG:NH2	1:A:791:GLN:O	2.32	0.63
1:B:886:ARG:NH1	1:B:1047:VAL:O	2.32	0.63
1:B:1725:GLN:NE2	1:B:1760:LEU:O	2.31	0.63
1:B:118:TYR:OH	1:B:181:ASP:OD2	2.16	0.63
1:B:801:ARG:NH2	1:B:984:ASP:OD1	2.24	0.62
1:D:749:ASP:O	1:D:753:GLN:NE2	2.32	0.62
1:C:510:ARG:NH2	3:C:3002:I3P:O51	2.32	0.62
1:A:1889:GLN:NE2	1:A:1946:GLU:O	2.32	0.62
1:C:611:THR:OG1	1:C:614:GLU:OE1	2.10	0.62
1:A:195:HIS:ND1	1:A:196:ALA:O	2.33	0.61
1:A:2394:ASP:OD1	1:A:2481:ARG:NH2	2.32	0.61
1:B:2394:ASP:OD1	1:B:2481:ARG:NH2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1735:LYS:NZ	1:C:1739:ASP:OD2	2.24	0.60
1:C:2006:SER:OG	1:C:2134:GLU:OE1	2.12	0.60
1:B:195:HIS:ND1	1:B:196:ALA:O	2.34	0.60
1:C:568:ARG:NH2	1:C:572:GLU:OE2	2.35	0.60
1:B:1949:GLN:NE2	1:B:2583:TYR:O	2.35	0.60
1:D:1194:GLN:NE2	1:D:1234:LYS:O	2.35	0.60
1:A:663:ASP:OD1	1:A:697:THR:OG1	2.10	0.60
1:D:533:GLY:N	1:D:536:VAL:O	2.34	0.60
1:C:1769:GLN:NE2	1:C:1879:LEU:O	2.35	0.60
1:A:1937:VAL:O	1:A:1940:THR:OG1	2.16	0.59
1:C:2038:GLU:OE2	1:C:2042:SER:OG	2.20	0.59
1:C:1951:PRO:O	1:C:1956:GLN:NE2	2.36	0.59
1:D:1735:LYS:NZ	1:D:1739:ASP:OD2	2.20	0.59
1:C:127:MET:O	1:C:440:ARG:NH2	2.36	0.59
1:B:494:LEU:O	1:B:558:ARG:NH2	2.35	0.59
1:A:1890:ASN:OD1	1:A:1893:ARG:NH2	2.36	0.58
1:C:132:TYR:N	1:C:153:ASP:O	2.36	0.58
1:A:118:TYR:OH	1:A:181:ASP:OD2	2.21	0.58
1:B:745:TYR:OH	1:B:788:ARG:O	2.12	0.58
1:B:1783:GLU:OE1	1:B:1897:ASN:ND2	2.35	0.58
1:B:1890:ASN:OD1	1:B:1893:ARG:NH2	2.37	0.58
1:D:1951:PRO:O	1:D:1956:GLN:NE2	2.37	0.58
1:C:1235:PHE:O	1:C:1242:ASN:ND2	2.36	0.57
1:B:663:ASP:OD1	1:B:697:THR:OG1	2.11	0.57
1:C:401:THR:OG1	1:C:416:MET:O	2.19	0.57
1:C:632:ASP:O	1:C:635:SER:OG	2.16	0.57
1:B:1085:ARG:NH1	1:B:1613:GLU:OE2	2.38	0.57
1:C:743:ARG:NH1	1:C:788:ARG:O	2.37	0.57
1:D:801:ARG:NH2	1:D:984:ASP:OD1	2.39	0.56
1:A:428:ALA:HB3	1:D:170:LEU:HD22	1.88	0.56
1:D:127:MET:O	1:D:440:ARG:NH2	2.39	0.56
1:D:827:LYS:O	1:D:831:ALA:N	2.39	0.56
1:C:1109:VAL:O	1:C:1113:GLU:N	2.38	0.56
1:D:132:TYR:N	1:D:153:ASP:O	2.38	0.56
1:A:1956:GLN:NE2	1:A:2002:ALA:O	2.40	0.55
1:D:1945:THR:O	1:D:1949:GLN:N	2.40	0.55
1:A:2523:LEU:O	1:A:2527:LYS:N	2.39	0.55
1:D:389:LEU:HB2	1:D:398:ILE:HD12	1.88	0.55
1:C:1945:THR:O	1:C:1949:GLN:N	2.38	0.55
1:B:1893:ARG:NH1	1:B:1955:ASN:OD1	2.39	0.55
1:C:2124:ILE:HD12	1:C:2138:PHE:HE1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1490:ALA:O	1:A:1494:LYS:N	2.41	0.54
1:A:1783:GLU:OE1	1:A:1897:ASN:ND2	2.40	0.54
1:B:888:LEU:HD21	1:B:971:ILE:HG23	1.90	0.54
1:A:1725:GLN:NE2	1:A:1760:LEU:O	2.41	0.54
1:A:656:VAL:HG13	1:A:657:LEU:HD22	1.89	0.54
1:A:1893:ARG:NH1	1:A:1955:ASN:OD1	2.40	0.54
1:A:1891:PHE:O	1:A:1895:GLN:NE2	2.41	0.53
1:D:482:PHE:O	1:D:505:ARG:NH1	2.42	0.53
1:D:2124:ILE:HD12	1:D:2138:PHE:HE1	1.74	0.53
1:C:153:ASP:OD2	1:C:156:GLY:N	2.41	0.53
1:C:1085:ARG:NH1	1:C:1613:GLU:OE2	2.42	0.53
1:C:494:LEU:O	1:C:558:ARG:NH2	2.41	0.53
1:B:656:VAL:HG13	1:B:657:LEU:HD22	1.90	0.53
1:D:2038:GLU:OE2	1:D:2042:SER:OG	2.25	0.53
1:D:153:ASP:OD2	1:D:156:GLY:N	2.42	0.52
1:D:1109:VAL:O	1:D:1113:GLU:N	2.42	0.52
1:D:1773:HIS:NE2	1:D:1777:MET:SD	2.82	0.52
1:D:1030:GLU:OE2	1:D:1605:ARG:NH2	2.43	0.52
1:C:305:ARG:NH2	1:C:365:SER:O	2.43	0.52
1:A:1397:VAL:O	1:A:1401:THR:OG1	2.16	0.52
1:B:2047:ARG:O	1:B:2051:HIS:ND1	2.42	0.51
1:B:1968:ASP:OD1	1:B:2019:SER:OG	2.27	0.51
1:C:389:LEU:HB2	1:C:398:ILE:HD12	1.91	0.51
1:C:1411:MET:O	1:C:1415:ASN:ND2	2.43	0.51
1:A:17:TYR:O	1:A:220:LYS:N	2.44	0.51
1:C:2394:ASP:OD1	1:C:2481:ARG:NH2	2.43	0.51
1:A:132:TYR:N	1:A:153:ASP:O	2.44	0.51
1:D:401:THR:OG1	1:D:416:MET:O	2.24	0.51
1:D:1322:MET:O	1:D:1326:THR:OG1	2.18	0.51
1:D:743:ARG:NH1	1:D:788:ARG:O	2.44	0.51
1:A:494:LEU:O	1:A:558:ARG:NE	2.45	0.50
1:A:568:ARG:NH1	3:A:3002:I3P:O3	2.44	0.50
1:B:1891:PHE:O	1:B:1895:GLN:NE2	2.44	0.50
1:D:838:GLU:OE2	1:D:883:ARG:NH1	2.45	0.50
1:D:563:SER:O	1:D:570:ASN:ND2	2.44	0.50
1:B:2367:ARG:NE	1:C:2352:GLU:OE2	2.44	0.50
1:D:640:SER:O	1:D:643:ILE:N	2.44	0.50
1:B:1956:GLN:NE2	1:B:2002:ALA:O	2.45	0.50
1:A:1878:GLN:OE1	1:A:1939:GLN:NE2	2.43	0.50
1:C:533:GLY:N	1:C:536:VAL:O	2.45	0.49
1:D:632:ASP:O	1:D:635:SER:OG	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1223:GLU:OE1	1:B:1226:ARG:NH2	2.46	0.49
1:C:667:ARG:NH2	1:C:669:GLU:OE2	2.46	0.49
1:D:126:HIS:O	1:D:130:ASN:N	2.44	0.49
1:C:482:PHE:O	1:C:505:ARG:NH1	2.44	0.49
1:D:446:ASN:OD1	1:D:512:GLN:OE1	2.31	0.49
1:A:1254:LEU:O	1:A:1285:HIS:NE2	2.46	0.49
1:D:31:LEU:O	1:D:131:LYS:NZ	2.46	0.49
1:C:886:ARG:NH1	1:C:1046:GLU:O	2.46	0.49
1:A:314:TYR:N	1:A:357:VAL:O	2.42	0.49
1:C:1116:ARG:O	1:C:1119:THR:OG1	2.27	0.49
1:A:428:ALA:HB3	1:D:170:LEU:CD2	2.43	0.48
1:B:305:ARG:NE	1:B:360:GLY:O	2.46	0.48
1:A:305:ARG:NE	1:A:360:GLY:O	2.46	0.48
1:D:305:ARG:NH2	1:D:365:SER:O	2.46	0.48
1:A:1787:LYS:NZ	1:A:1791:ASP:OD2	2.45	0.48
1:B:1254:LEU:O	1:B:1285:HIS:NE2	2.47	0.48
1:A:1981:LEU:O	1:A:1985:ARG:N	2.44	0.48
1:D:118:TYR:OH	1:D:181:ASP:OD2	2.32	0.48
1:C:126:HIS:O	1:C:130:ASN:N	2.44	0.48
1:D:1878:GLN:OE1	1:D:1939:GLN:NE2	2.44	0.48
1:D:2401:ARG:NE	1:D:2449:ASP:OD2	2.47	0.48
1:A:1223:GLU:OE1	1:A:1226:ARG:NH2	2.47	0.48
1:A:1337:ASN:OD1	1:A:1338:ASP:N	2.47	0.47
1:A:2047:ARG:O	1:A:2051:HIS:ND1	2.46	0.47
1:B:132:TYR:N	1:B:153:ASP:O	2.48	0.47
1:B:965:MET:SD	1:B:1065:HIS:ND1	2.87	0.47
1:D:466:GLN:OE1	1:D:469:ARG:NH2	2.46	0.47
1:C:640:SER:O	1:C:643:ILE:N	2.44	0.47
1:B:1033:GLU:OE2	1:B:1085:ARG:NH2	2.48	0.47
1:D:2192:PRO:O	1:D:2196:TRP:N	2.46	0.47
1:B:255:ASP:OD1	1:B:256:GLU:N	2.48	0.47
1:B:1053:ARG:NH1	1:B:1694:TYR:O	2.47	0.47
1:B:1337:ASN:OD1	1:B:1338:ASP:N	2.48	0.47
1:B:1981:LEU:O	1:B:1985:ARG:N	2.43	0.47
1:C:446:ASN:OD1	1:C:512:GLN:OE1	2.33	0.47
1:B:114:ASP:OD1	1:B:115:VAL:N	2.48	0.47
1:B:561:ARG:NH1	1:B:593:ASP:O	2.48	0.47
1:D:2003:LEU:O	1:D:2012:ASN:ND2	2.48	0.47
1:A:1033:GLU:OE2	1:A:1085:ARG:NH2	2.48	0.47
1:C:1053:ARG:NE	1:C:1693:ASN:O	2.47	0.47
1:A:391:HIS:O	1:A:395:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ASP:OD1	1:A:1049:ASP:N	2.48	0.47
1:A:1095:VAL:O	1:A:1195:ARG:NH2	2.48	0.47
1:A:640:SER:O	1:A:643:ILE:N	2.46	0.46
1:D:1085:ARG:NH1	1:D:1613:GLU:OE2	2.49	0.46
1:C:1932:ASP:OD1	1:C:1933:ASN:N	2.48	0.46
1:A:255:ASP:OD1	1:A:256:GLU:N	2.48	0.46
1:A:2518:ASP:OD2	1:B:2524:ARG:NE	2.42	0.46
1:D:2114:LEU:O	1:D:2118:GLU:N	2.49	0.46
1:C:838:GLU:OE2	1:C:883:ARG:NH1	2.48	0.46
1:C:1048:ASP:OD1	1:C:1049:ASP:N	2.49	0.46
1:A:1932:ASP:OD1	1:A:1933:ASN:N	2.48	0.46
1:D:1370:ASP:O	1:D:1374:ALA:N	2.47	0.46
1:B:640:SER:O	1:B:643:ILE:N	2.46	0.46
1:B:1048:ASP:OD1	1:B:1049:ASP:N	2.48	0.46
1:B:2558:HIS:ND1	1:B:2562:GLU:OE1	2.46	0.46
1:D:2549:ASP:OD1	1:D:2550:ASN:N	2.48	0.46
1:B:2523:LEU:O	1:B:2527:LYS:N	2.43	0.46
1:D:667:ARG:NH2	1:D:669:GLU:OE2	2.48	0.46
1:A:568:ARG:NH2	3:A:3002:I3P:O11	2.49	0.46
1:A:814:ASP:O	1:A:817:SER:OG	2.27	0.46
1:A:632:ASP:O	1:A:635:SER:OG	2.20	0.46
1:A:1930:ASN:OD1	1:A:1931:GLU:N	2.49	0.46
1:D:1048:ASP:OD1	1:D:1049:ASP:N	2.48	0.46
1:D:1769:GLN:NE2	1:D:1879:LEU:O	2.49	0.46
1:B:1932:ASP:OD1	1:B:1933:ASN:N	2.49	0.46
1:C:164:ILE:HG23	1:C:164:ILE:O	2.17	0.45
1:C:1764:GLY:O	1:C:1883:ASN:ND2	2.49	0.45
1:B:104:ASN:OD1	1:B:105:ASP:N	2.49	0.45
1:C:2549:ASP:OD1	1:C:2550:ASN:N	2.49	0.45
1:D:1033:GLU:OE2	1:D:1085:ARG:NH2	2.48	0.45
1:B:1878:GLN:OE1	1:B:1939:GLN:NE2	2.46	0.45
1:D:1116:ARG:O	1:D:1119:THR:OG1	2.31	0.45
1:D:1932:ASP:OD1	1:D:1933:ASN:N	2.49	0.45
1:C:803:TRP:N	1:C:1098:LEU:O	2.50	0.45
1:C:838:GLU:O	1:C:842:ASN:ND2	2.49	0.45
1:A:217:THR:HG1	1:A:219:TRP:HE1	1.64	0.45
1:B:17:TYR:O	1:B:220:LYS:N	2.50	0.45
1:A:32:VAL:HG12	1:A:32:VAL:O	2.17	0.45
1:D:164:ILE:HG23	1:D:164:ILE:O	2.17	0.45
1:B:314:TYR:N	1:B:357:VAL:O	2.44	0.45
1:A:541:LEU:O	1:A:550:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ASP:OD1	1:A:759:LEU:N	2.50	0.44
1:B:32:VAL:HG12	1:B:32:VAL:O	2.17	0.44
1:C:2192:PRO:O	1:C:2196:TRP:N	2.49	0.44
1:C:1322:MET:O	1:C:1326:THR:OG1	2.22	0.44
1:C:730:ARG:NH2	1:C:772:ASP:OD2	2.50	0.44
1:C:1912:ASP:O	1:C:1916:GLY:N	2.51	0.44
1:C:2114:LEU:O	1:C:2118:GLU:N	2.50	0.44
1:B:758:ASP:OD1	1:B:759:LEU:N	2.50	0.44
1:B:1787:LYS:NZ	1:B:1791:ASP:OD2	2.50	0.44
1:B:1930:ASN:OD1	1:B:1931:GLU:N	2.50	0.44
1:C:758:ASP:OD1	1:C:759:LEU:N	2.51	0.44
1:A:153:ASP:OD2	1:A:156:GLY:N	2.46	0.44
1:D:557:TYR:OH	1:D:584:GLN:OE1	2.36	0.44
1:D:719:ASN:ND2	1:D:722:ASP:OD2	2.51	0.44
1:D:2124:ILE:HD11	1:D:2567:ASN:O	2.18	0.44
1:C:1350:LYS:O	1:C:1353:ARG:NH1	2.50	0.44
1:C:1725:GLN:NE2	1:C:1759:HIS:O	2.51	0.44
1:A:988:SER:O	1:A:992:SER:OG	2.29	0.43
1:A:1897:ASN:OD1	1:A:1898:LYS:N	2.51	0.43
1:B:1897:ASN:OD1	1:B:1898:LYS:N	2.52	0.43
1:B:1115:ASP:OD1	1:B:1116:ARG:N	2.51	0.43
1:B:1397:VAL:O	1:B:1401:THR:OG1	2.14	0.43
1:C:1878:GLN:OE1	1:C:1939:GLN:NE2	2.42	0.43
1:C:2124:ILE:HD11	1:C:2567:ASN:O	2.19	0.43
1:A:1103:ASP:O	1:A:1107:TYR:N	2.51	0.43
1:A:2558:HIS:ND1	1:A:2562:GLU:OE1	2.46	0.43
1:A:114:ASP:OD1	1:A:115:VAL:N	2.49	0.43
1:A:237:GLY:N	1:A:296:GLY:O	2.50	0.43
1:A:60:CYS:O	1:A:123:GLN:N	2.52	0.43
1:B:568:ARG:NH2	3:B:3002:I3P:O11	2.51	0.43
1:A:764:MET:O	1:A:774:ARG:NH2	2.51	0.43
1:B:1987:ASP:OD1	1:B:1988:LEU:N	2.52	0.43
1:D:44:ASP:OD1	1:D:45:LEU:N	2.51	0.43
1:A:239:ASP:OD1	1:A:240:VAL:N	2.52	0.42
1:D:1670:GLN:NE2	1:D:1752:GLU:OE1	2.52	0.42
1:C:394:THR:HG1	1:C:396:THR:CB	2.31	0.42
1:C:1953:HIS:NE2	1:C:2006:SER:O	2.48	0.42
1:D:838:GLU:O	1:D:842:ASN:ND2	2.51	0.42
1:C:864:VAL:O	1:C:868:HIS:N	2.49	0.42
1:C:118:TYR:OH	1:C:181:ASP:OD2	2.37	0.42
1:B:1098:LEU:HD22	1:B:1103:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1309:ALA:HB3	1:B:1312:LYS:O	2.20	0.42
1:A:2225:TYR:OH	1:A:2278:ILE:HG21	2.19	0.42
1:B:111:VAL:HG12	1:B:111:VAL:O	2.20	0.42
1:B:277:THR:HG23	1:B:277:THR:O	2.20	0.42
1:D:1764:GLY:O	1:D:1883:ASN:ND2	2.52	0.42
1:D:1912:ASP:O	1:D:1916:GLY:N	2.53	0.42
1:C:471:PHE:O	1:C:475:LEU:N	2.51	0.42
1:B:1887:ASP:O	1:B:1891:PHE:N	2.50	0.42
1:C:44:ASP:OD1	1:C:45:LEU:N	2.53	0.42
1:A:1427:GLU:HG3	1:D:138:ARG:HH12	1.85	0.42
1:B:1043:SER:OG	1:B:1044:MET:N	2.52	0.42
1:B:2592:GLN:O	1:B:2596:ASN:OD1	2.38	0.42
1:C:872:TYR:OH	1:C:973:GLU:O	2.37	0.42
1:A:242:ARG:NH2	1:A:277:THR:OG1	2.52	0.42
1:A:1115:ASP:OD1	1:A:1116:ARG:N	2.52	0.42
1:A:1945:THR:O	1:A:1949:GLN:N	2.44	0.42
1:B:391:HIS:O	1:B:395:ASN:N	2.53	0.42
1:B:2319:GLU:O	1:B:2323:HIS:ND1	2.48	0.42
1:A:543:ASP:OD2	1:A:545:LYS:NZ	2.53	0.42
1:A:1968:ASP:OD1	1:A:2019:SER:OG	2.31	0.42
1:B:632:ASP:O	1:B:635:SER:OG	2.25	0.42
1:D:255:ASP:OD1	1:D:256:GLU:N	2.53	0.42
1:D:2358:VAL:O	1:D:2361:SER:OG	2.29	0.42
1:A:1987:ASP:OD1	1:A:1988:LEU:N	2.52	0.42
1:C:192:GLN:NE2	1:C:214:ASN:OD1	2.52	0.42
1:C:1681:ASP:OD1	1:C:1682:ARG:N	2.52	0.42
1:A:104:ASN:OD1	1:A:105:ASP:N	2.53	0.41
1:A:1081:HIS:O	1:A:1084:GLN:NE2	2.53	0.41
1:A:2319:GLU:O	1:A:2323:HIS:ND1	2.47	0.41
1:D:1127:TRP:O	1:D:1169:TYR:OH	2.27	0.41
1:D:758:ASP:OD1	1:D:759:LEU:N	2.53	0.41
1:D:1043:SER:OG	1:D:1044:MET:N	2.53	0.41
1:D:1681:ASP:OD1	1:D:1682:ARG:N	2.53	0.41
1:A:2123:GLN:OE1	1:A:2135:GLN:OE1	2.38	0.41
1:A:2592:GLN:O	1:A:2596:ASN:OD1	2.39	0.41
1:C:239:ASP:OD1	1:C:240:VAL:N	2.53	0.41
1:C:2129:GLN:N	1:C:2589:TYR:OH	2.53	0.41
1:A:434:VAL:HG11	1:A:439:ILE:HD11	2.02	0.41
1:B:239:ASP:OD1	1:B:240:VAL:N	2.54	0.41
1:D:314:TYR:O	1:D:357:VAL:N	2.53	0.41
1:D:1787:LYS:NZ	1:D:1791:ASP:OD2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:SER:OG	1:C:466:GLN:N	2.53	0.41
1:C:75:LYS:NZ	1:C:489:ASN:O	2.52	0.41
1:B:2549:ASP:OD1	1:B:2550:ASN:N	2.54	0.41
1:C:86:ASP:OD1	1:C:87:VAL:N	2.54	0.41
1:A:277:THR:HG23	1:A:277:THR:O	2.20	0.41
1:B:1490:ALA:O	1:B:1494:LYS:N	2.53	0.41
1:A:111:VAL:O	1:A:111:VAL:HG12	2.20	0.41
1:A:1309:ALA:HB3	1:A:1312:LYS:O	2.20	0.41
1:A:2024:GLU:N	1:A:2024:GLU:OE1	2.53	0.41
1:D:1225:LEU:O	1:D:1228:THR:OG1	2.32	0.41
1:D:1960:VAL:HG21	1:D:2012:ASN:OD1	2.21	0.41
1:C:1043:SER:OG	1:C:1044:MET:N	2.53	0.41
1:C:1749:ILE:O	1:C:1753:SER:OG	2.29	0.41
1:A:138:ARG:NH2	1:B:1427:GLU:OE2	2.54	0.41
1:C:238:GLY:N	1:C:285:VAL:O	2.52	0.41
1:A:666:ILE:HG22	1:A:732:GLN:HG2	2.04	0.40
1:B:237:GLY:N	1:B:296:GLY:O	2.49	0.40
1:B:2123:GLN:OE1	1:B:2135:GLN:OE1	2.39	0.40
1:D:465:SER:OG	1:D:466:GLN:N	2.55	0.40
1:D:1068:ALA:HB3	1:D:1069:PRO:HD3	2.03	0.40
1:A:245:HIS:N	1:A:250:LYS:O	2.51	0.40
1:B:1081:HIS:O	1:B:1084:GLN:NE2	2.53	0.40
1:B:1755:GLY:O	1:B:1759:HIS:ND1	2.49	0.40
1:B:1889:GLN:NE2	1:B:1946:GLU:O	2.55	0.40
1:D:2260:SER:OG	1:D:2261:ILE:N	2.54	0.40
1:A:2341:TYR:HD1	1:A:2344:LEU:HD11	1.87	0.40
1:B:63:ASN:O	1:B:161:TRP:NE1	2.52	0.40
1:C:2260:SER:OG	1:C:2261:ILE:N	2.55	0.40
1:A:63:ASN:O	1:A:161:TRP:NE1	2.51	0.40
1:B:772:ASP:OD1	1:B:773:LEU:N	2.54	0.40
1:C:1068:ALA:HB3	1:C:1069:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2148/2671 (80%)	2081 (97%)	67 (3%)	0	100	100
1	B	2148/2671 (80%)	2079 (97%)	69 (3%)	0	100	100
1	C	2144/2671 (80%)	2073 (97%)	71 (3%)	0	100	100
1	D	2144/2671 (80%)	2069 (96%)	75 (4%)	0	100	100
All	All	8584/10684 (80%)	8302 (97%)	282 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1924/2385 (81%)	1919 (100%)	5 (0%)	92	94
1	B	1924/2385 (81%)	1919 (100%)	5 (0%)	92	94
1	C	1879/2385 (79%)	1873 (100%)	6 (0%)	92	94
1	D	1879/2385 (79%)	1873 (100%)	6 (0%)	92	94
All	All	7606/9540 (80%)	7584 (100%)	22 (0%)	92	94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ARG
1	A	1106	ASN
1	A	2064	ASN
1	A	2289	ASN
1	A	2471	ARG
1	B	171	ARG
1	B	1106	ASN
1	B	2064	ASN
1	B	2289	ASN
1	B	2471	ARG

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Mol	Chain	Res	Type
1	D	320	ASN
1	D	390	ARG
1	D	1976	ASN
1	D	2289	ASN
1	D	2357	ASN
1	D	2472	ASN
1	C	320	ASN
1	C	390	ARG
1	C	1976	ASN
1	C	2289	ASN
1	C	2357	ASN
1	C	2472	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	I3P	C	3002	-	24,24,24	1.30	3 (12%)	36,39,39	0.65	0
3	I3P	A	3002	-	24,24,24	1.29	3 (12%)	36,39,39	0.58	0
3	I3P	B	3002	-	24,24,24	1.29	3 (12%)	36,39,39	0.58	0
3	I3P	D	3002	-	24,24,24	1.29	3 (12%)	36,39,39	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I3P	C	3002	-	-	4/15/39/39	0/1/1/1
3	I3P	A	3002	-	-	5/15/39/39	0/1/1/1
3	I3P	B	3002	-	-	1/15/39/39	0/1/1/1
3	I3P	D	3002	-	-	3/15/39/39	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	I3P	P4-O4	3.16	1.65	1.59
3	D	3002	I3P	P4-O4	3.14	1.65	1.59
3	C	3002	I3P	P1-O1	3.14	1.65	1.59
3	B	3002	I3P	P4-O4	3.14	1.65	1.59
3	D	3002	I3P	P1-O1	3.12	1.65	1.59
3	C	3002	I3P	P4-O4	3.11	1.65	1.59
3	B	3002	I3P	P1-O1	3.10	1.65	1.59
3	A	3002	I3P	P1-O1	3.09	1.65	1.59
3	C	3002	I3P	P5-O5	3.09	1.65	1.59
3	A	3002	I3P	P5-O5	3.08	1.65	1.59
3	D	3002	I3P	P5-O5	3.03	1.65	1.59
3	B	3002	I3P	P5-O5	3.03	1.65	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3002	I3P	C5-O5-P5-O51
3	B	3002	I3P	C5-O5-P5-O51

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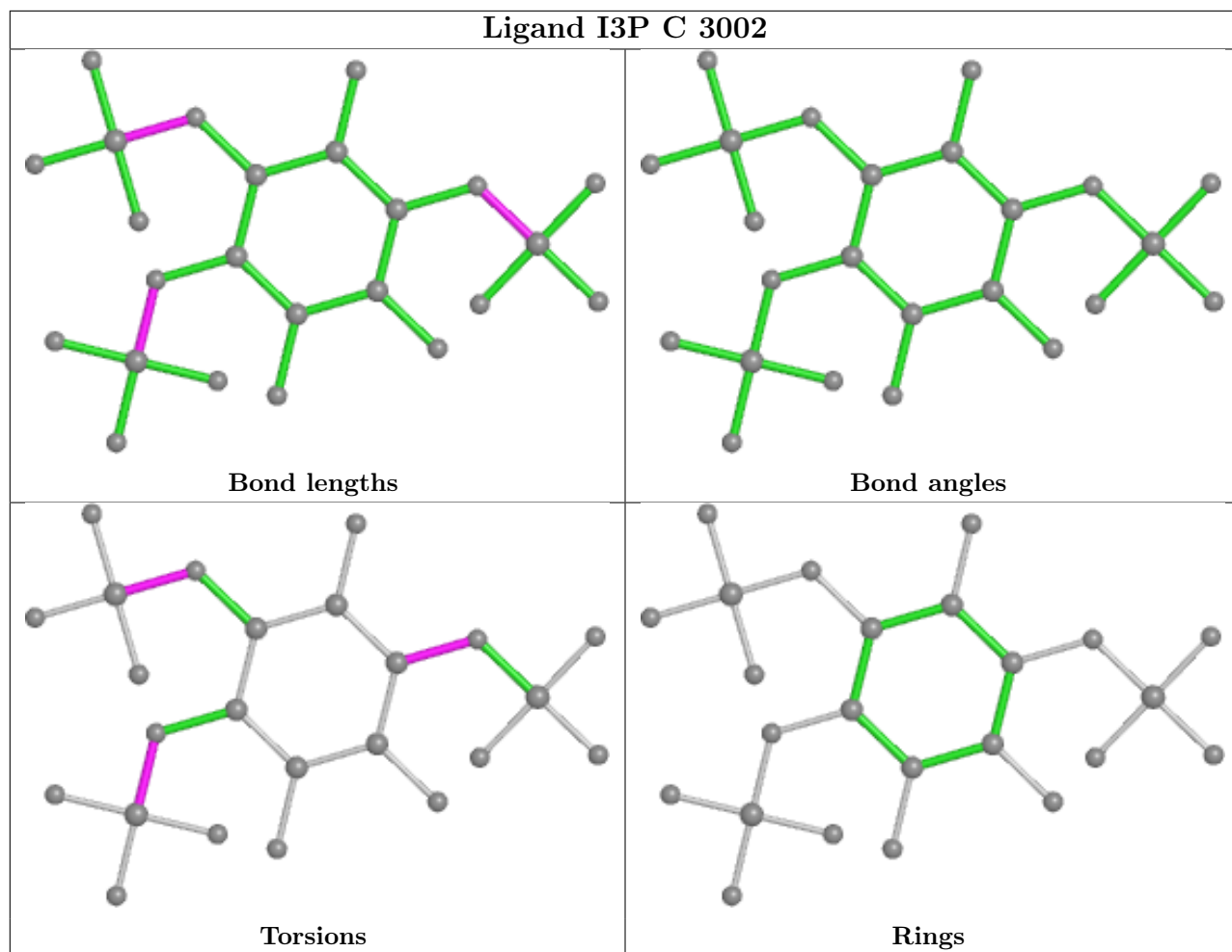
Mol	Chain	Res	Type	Atoms
3	D	3002	I3P	C5-O5-P5-O53
3	C	3002	I3P	C5-O5-P5-O53
3	C	3002	I3P	C5-O5-P5-O51
3	A	3002	I3P	C4-O4-P4-O42
3	A	3002	I3P	C1-O1-P1-O13
3	A	3002	I3P	C4-O4-P4-O43
3	A	3002	I3P	C5-O5-P5-O53
3	D	3002	I3P	C6-C1-O1-P1
3	D	3002	I3P	C4-O4-P4-O43
3	C	3002	I3P	C6-C1-O1-P1
3	C	3002	I3P	C4-O4-P4-O43

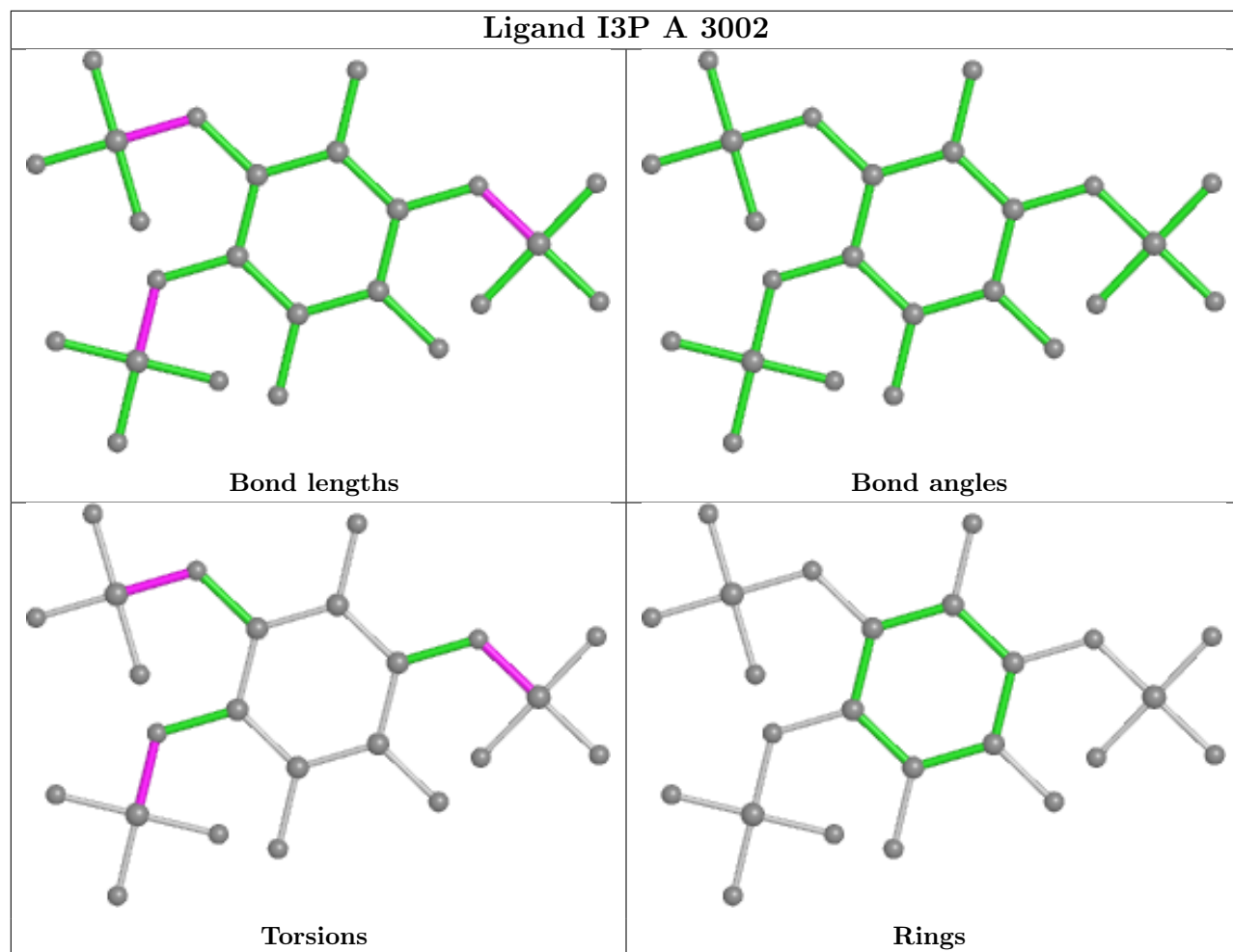
There are no ring outliers.

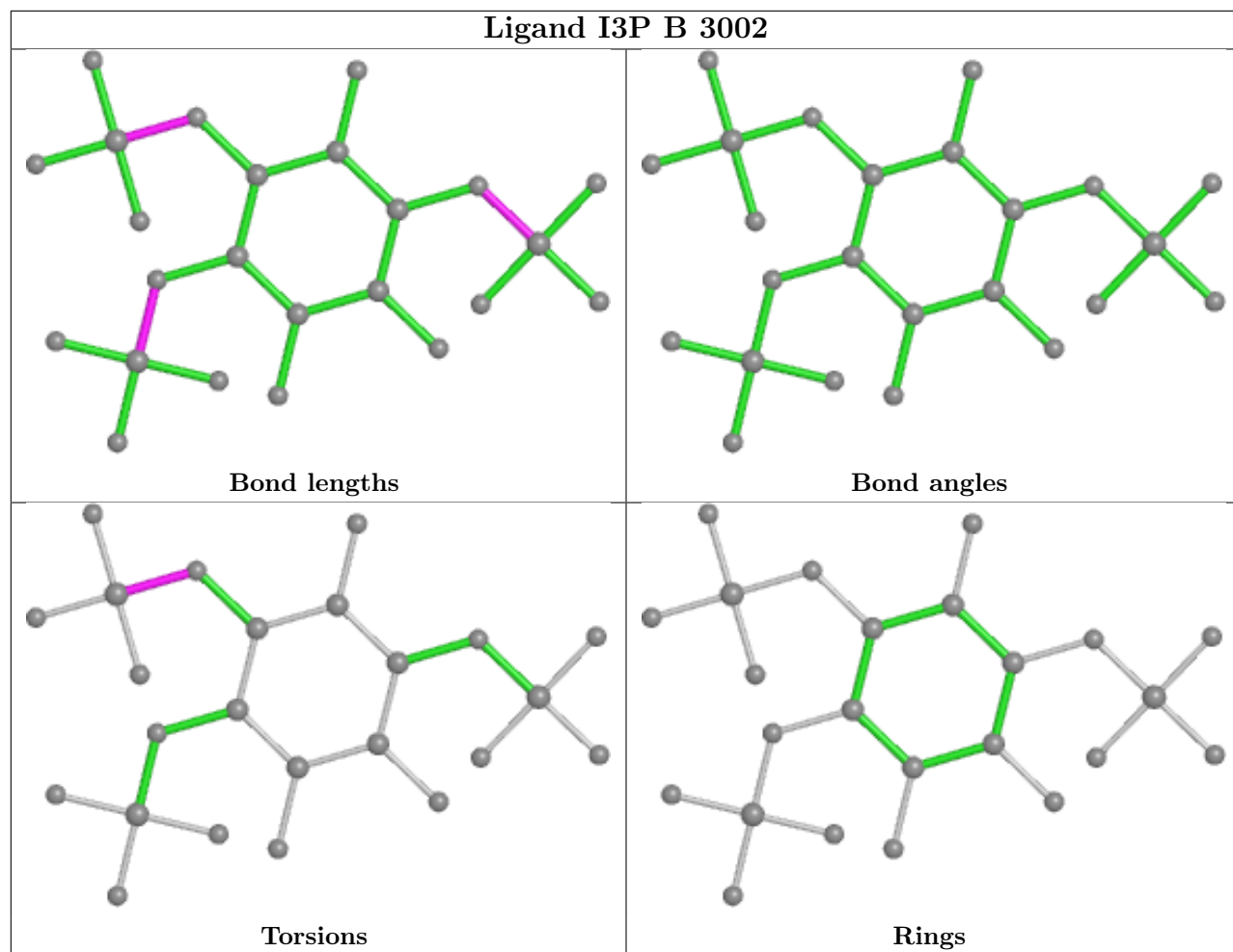
4 monomers are involved in 6 short contacts:

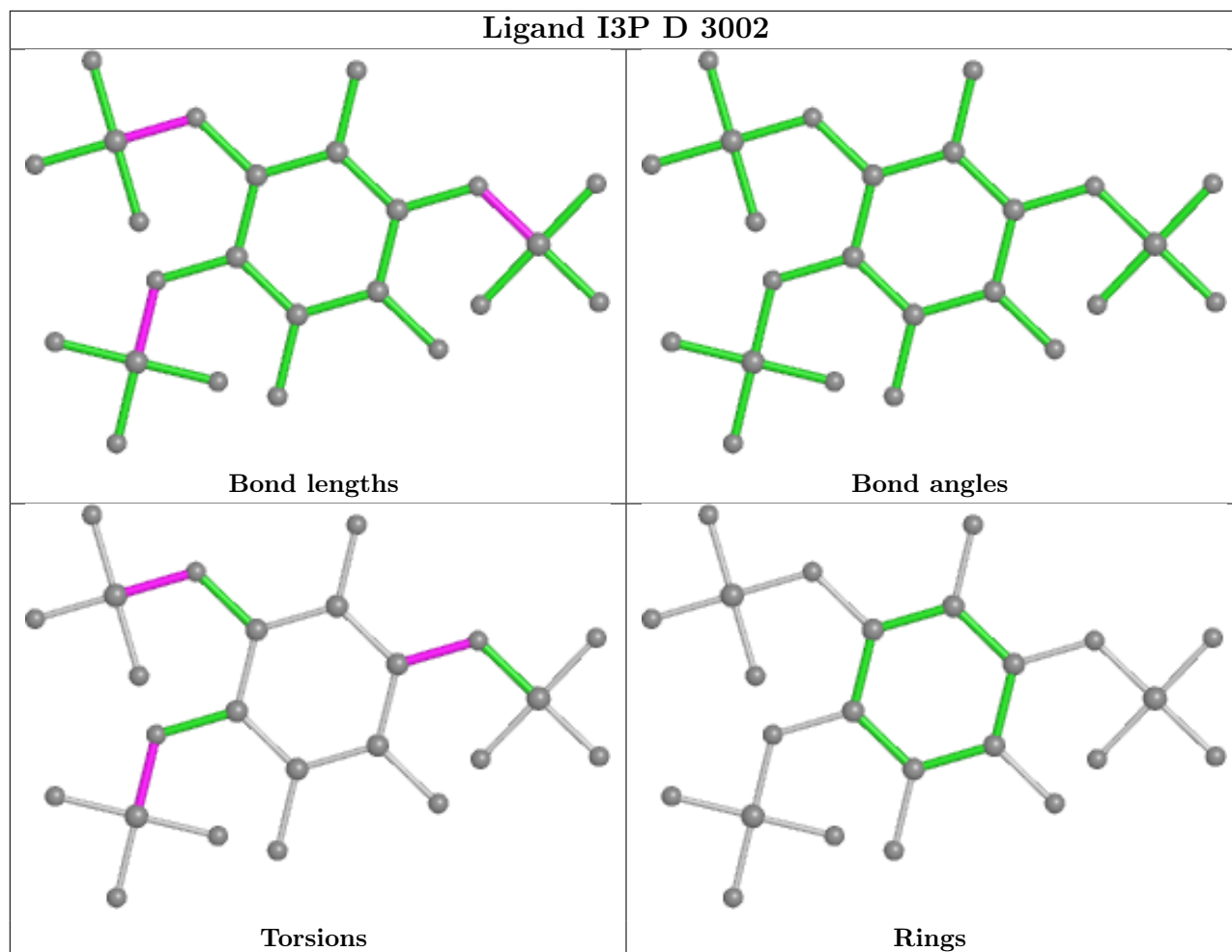
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3002	I3P	2	0
3	A	3002	I3P	2	0
3	B	3002	I3P	1	0
3	D	3002	I3P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	5
1	C	5
1	A	3
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1552:TRP	C	1587:ASP	N	49.50

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1552:TRP	C	1587:ASP	N	49.46
1	B	1552:TRP	C	1587:ASP	N	49.24
1	C	1552:TRP	C	1587:ASP	N	48.46
1	C	1484:ARG	C	1490:ALA	N	15.89
1	D	1484:ARG	C	1490:ALA	N	15.60
1	A	1533:ARG	C	1541:ALA	N	15.24
1	B	1533:ARG	C	1541:ALA	N	15.07
1	C	1533:ARG	C	1541:ALA	N	15.00
1	D	1533:ARG	C	1541:ALA	N	14.96
1	D	1508:GLY	C	1515:ALA	N	7.89
1	C	1508:GLY	C	1515:ALA	N	7.87
1	D	2252:TYR	C	2260:SER	N	6.94
1	C	2252:TYR	C	2260:SER	N	6.66
1	A	2252:TYR	C	2260:SER	N	6.12
1	B	2252:TYR	C	2260:SER	N	5.93

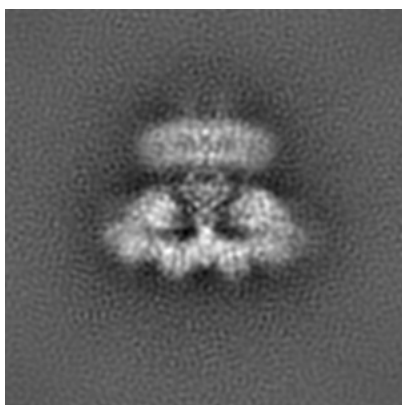
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7986. These allow visual inspection of the internal detail of the map and identification of artifacts.

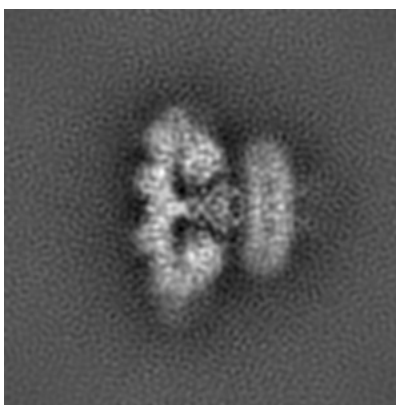
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

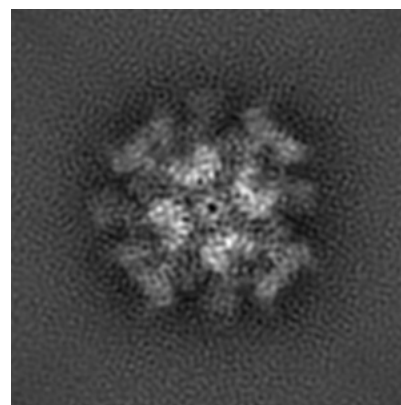
6.1.1 Primary map



X



Y

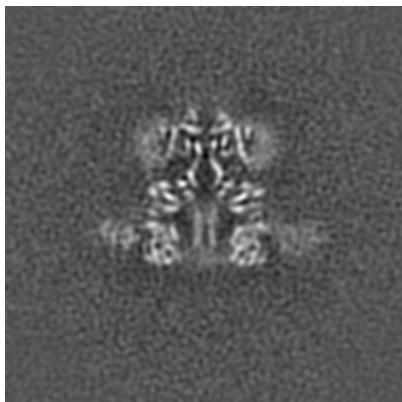


Z

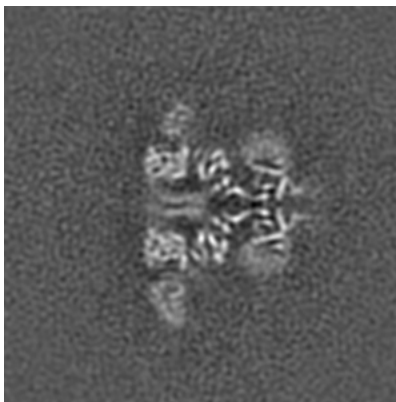
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

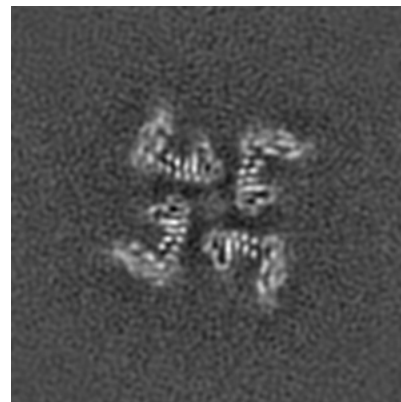
6.2.1 Primary map



X Index: 192



Y Index: 192

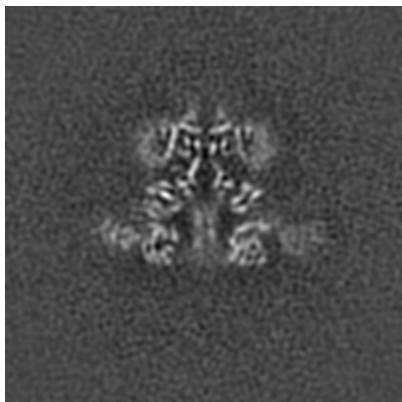


Z Index: 192

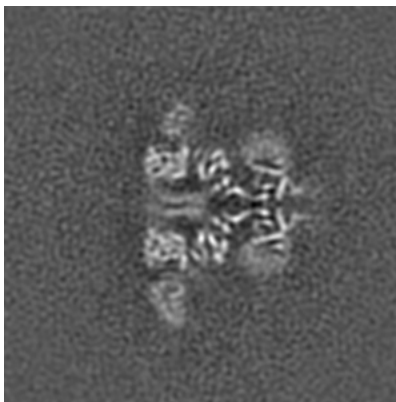
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

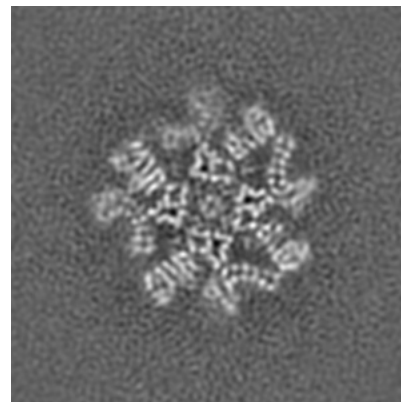
6.3.1 Primary map



X Index: 194



Y Index: 192

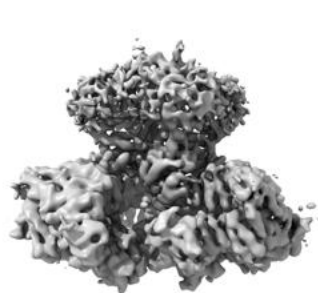


Z Index: 157

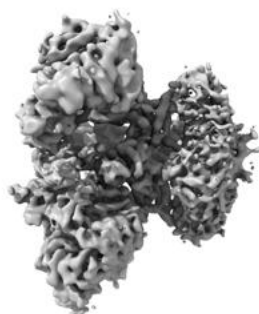
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.96. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

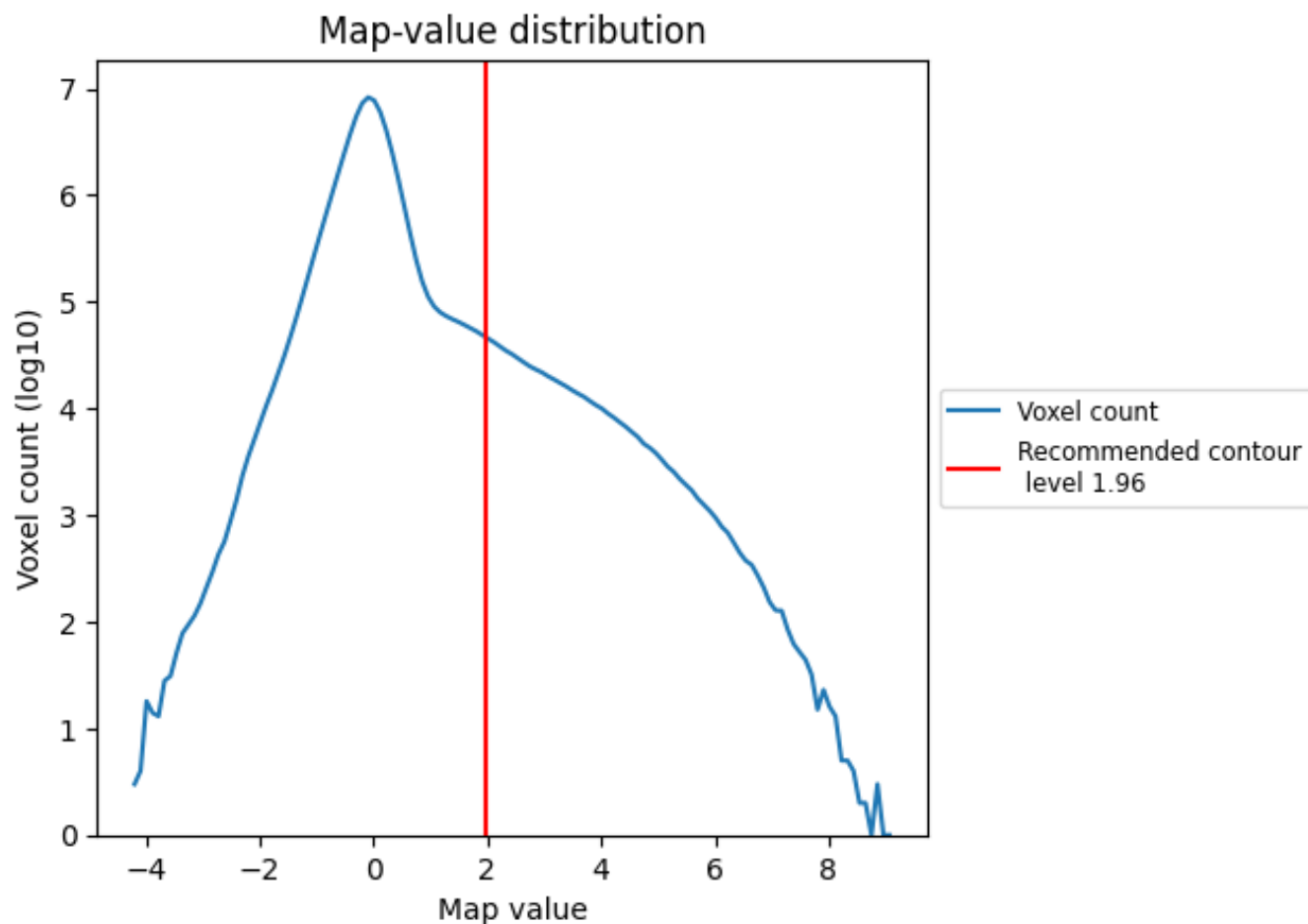
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

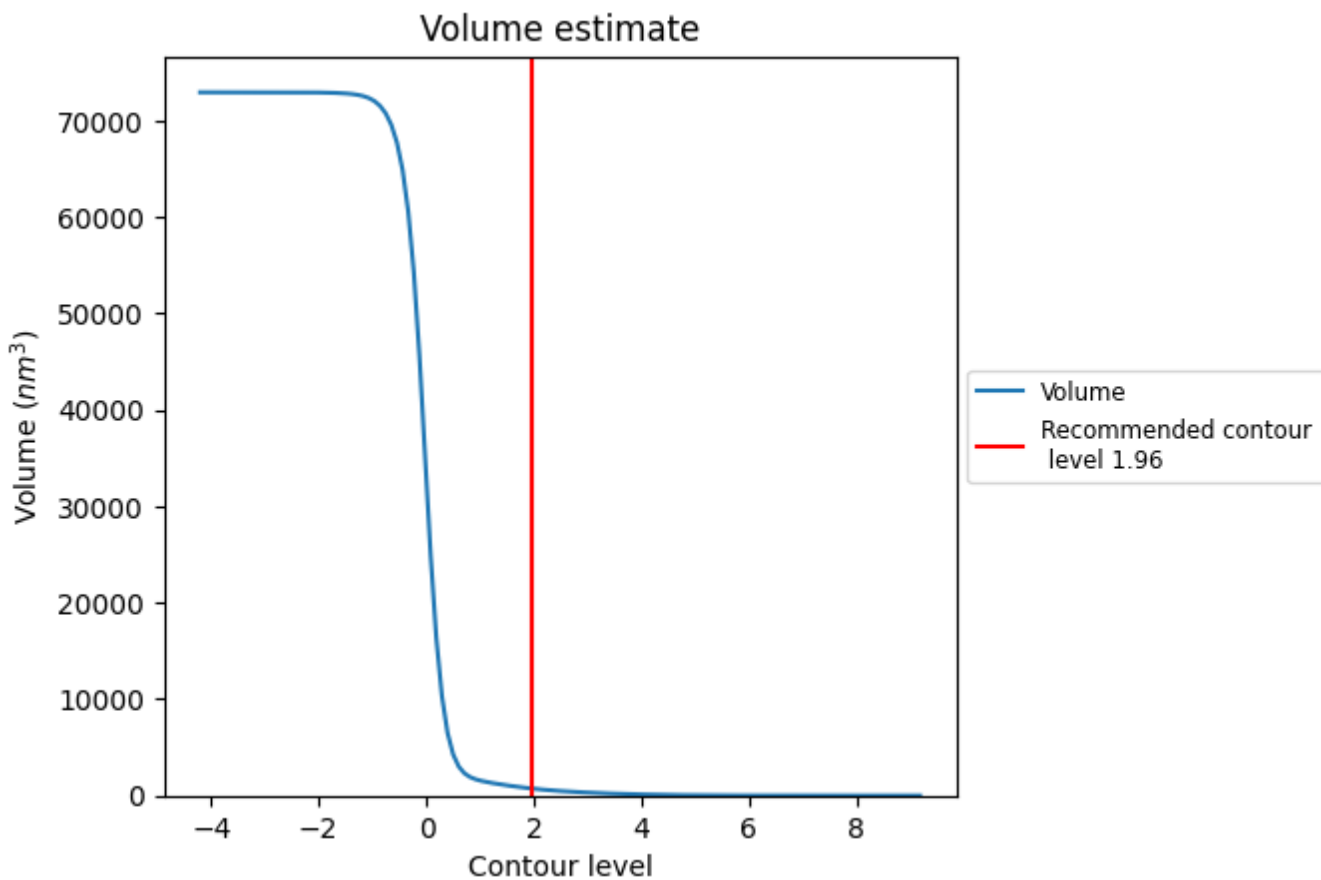
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

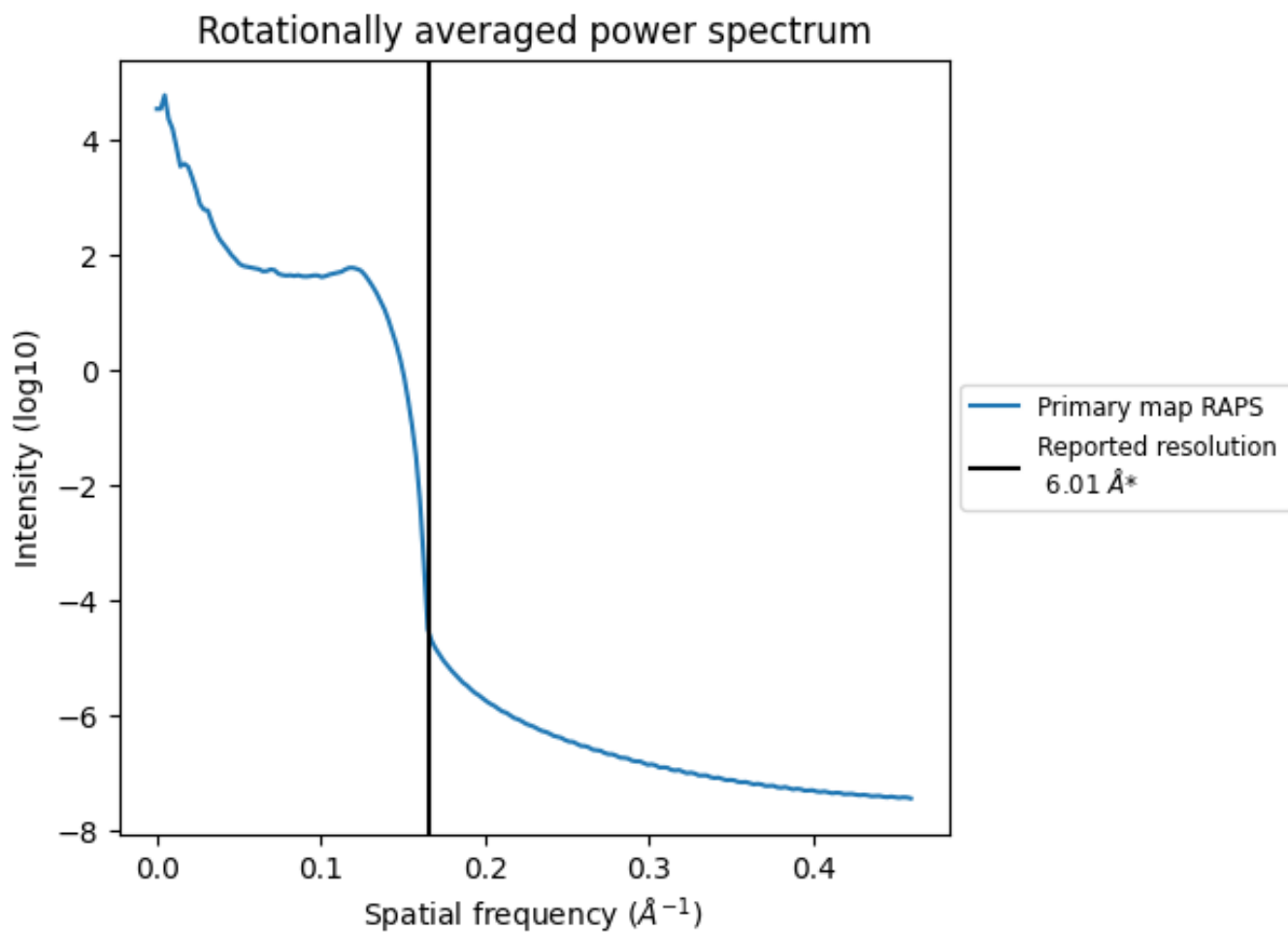
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 732 nm^3 ; this corresponds to an approximate mass of 661 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i



*Reported resolution corresponds to spatial frequency of 0.166 Å⁻¹

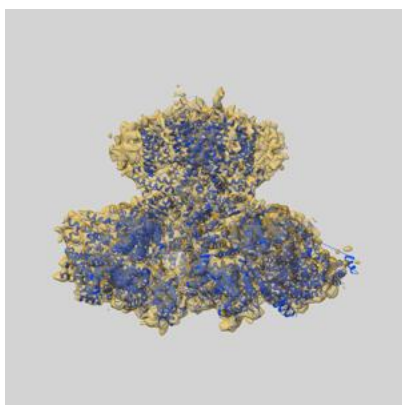
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

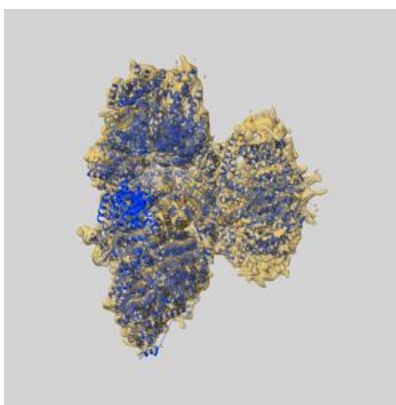
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7986 and PDB model 6DQZ. Per-residue inclusion information can be found in section 3 on page 5.

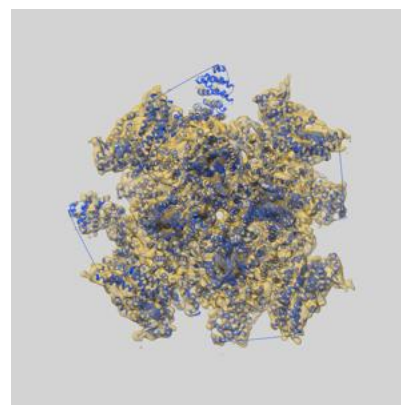
9.1 Map-model overlay [i](#)



X



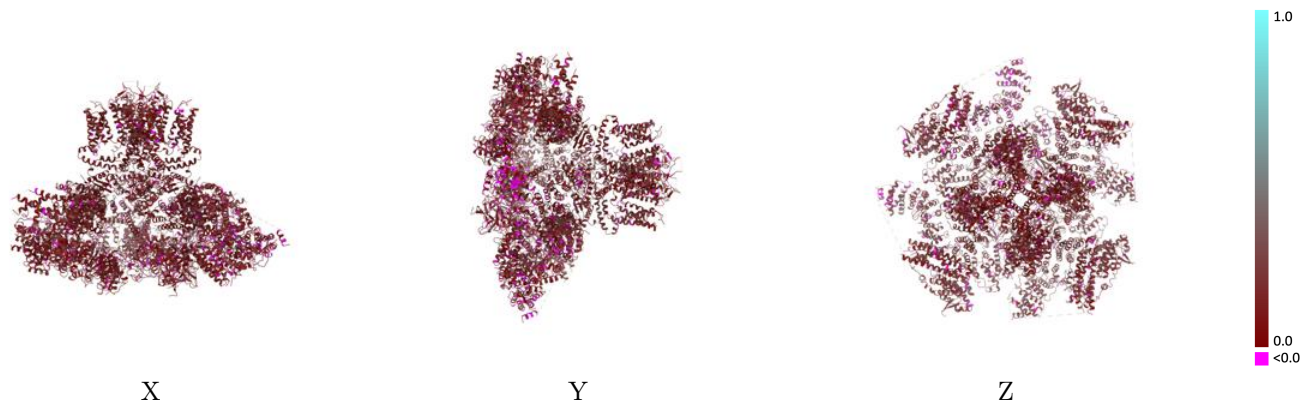
Y



Z

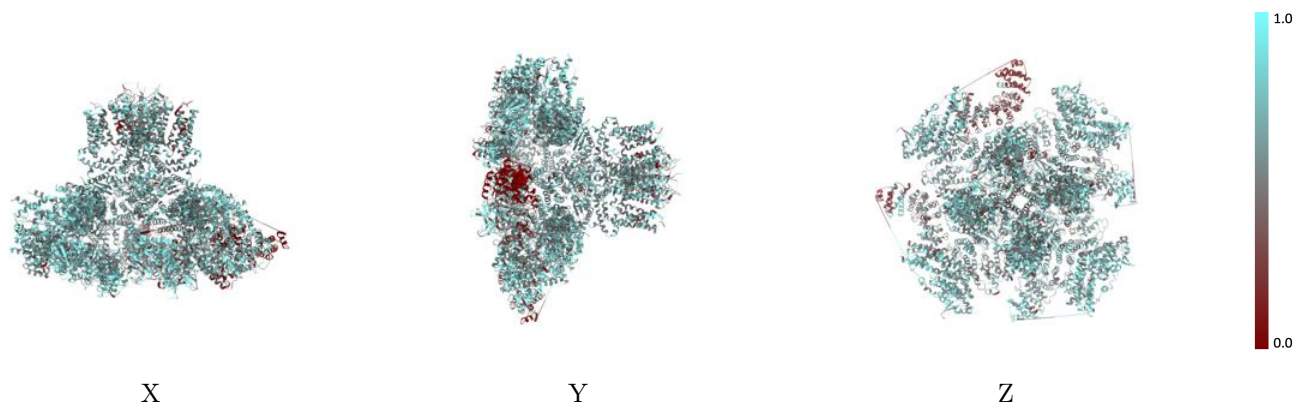
The images above show the 3D surface view of the map at the recommended contour level 1.96 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



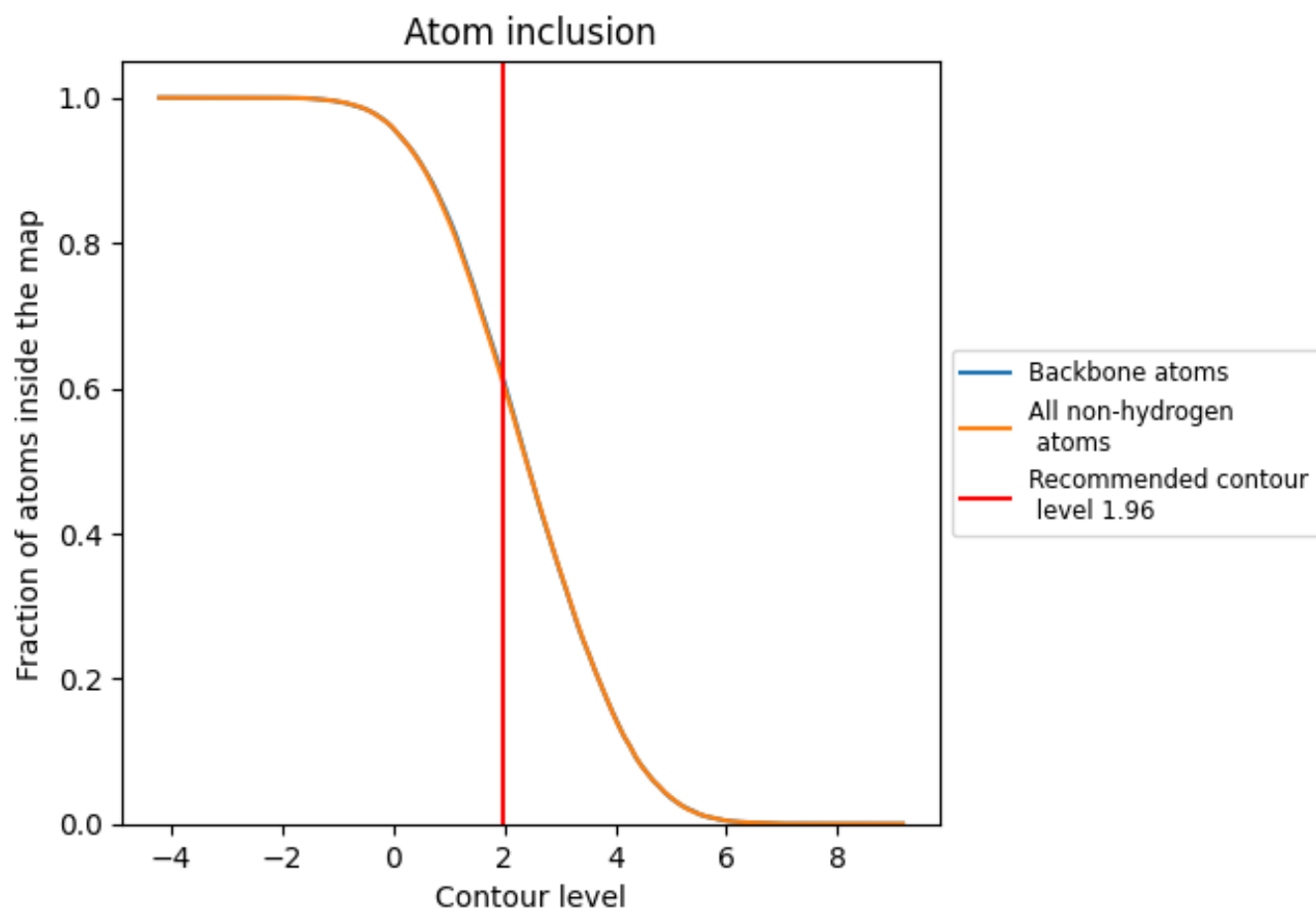
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.96).











9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (1.96) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6131	 0.1510
A	 0.6489	 0.1570
B	 0.6290	 0.1550
C	 0.5725	 0.1450
D	 0.6250	 0.1500

